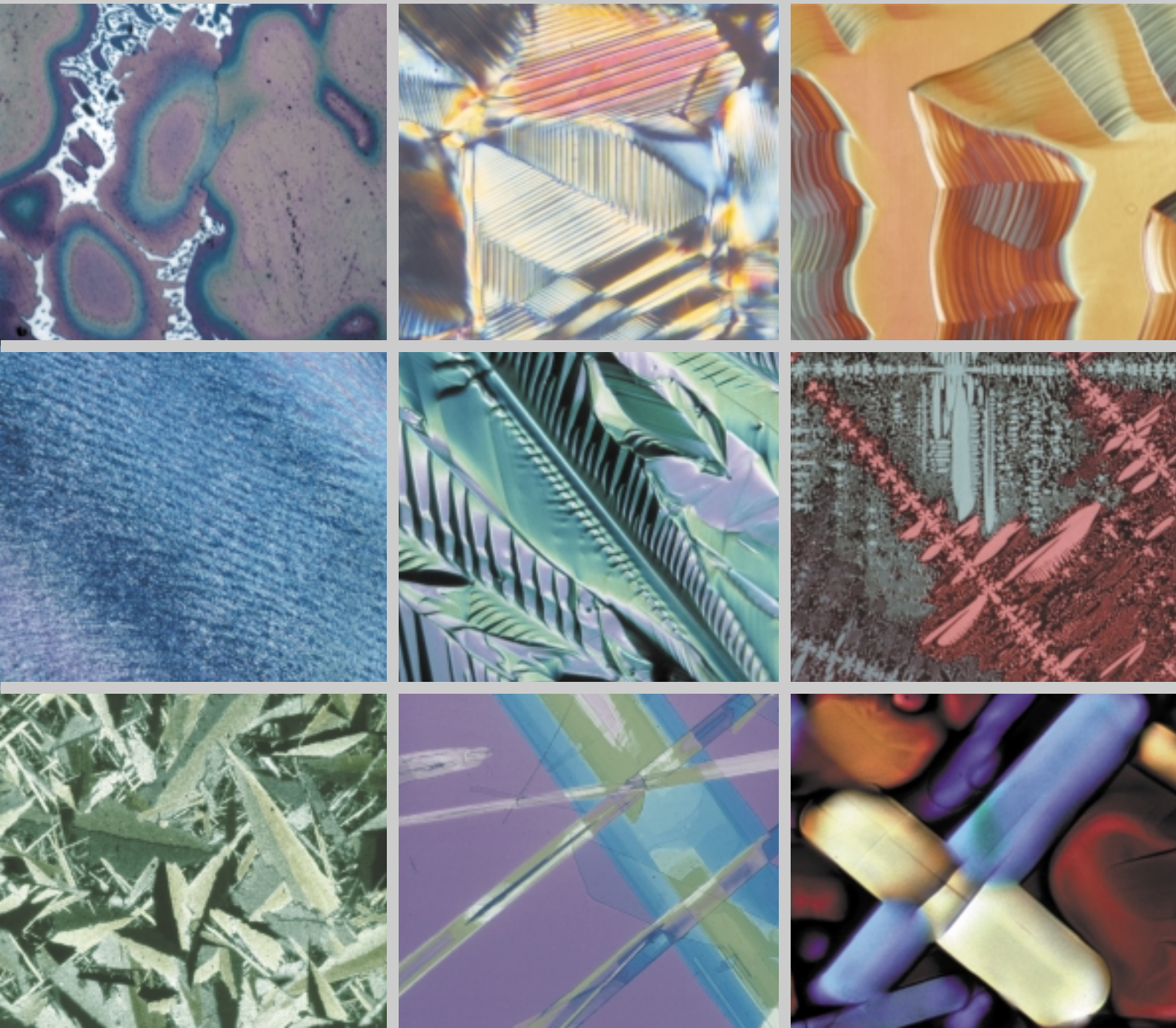
MAX-PLANCK-GESELLSCHAFT

EUROPEAN WHITE BOOK

ON FUNDAMENTAL RESEARCH IN MATERIALS SCIENCE

MAX-PLANCK-INSTITUT FÜR METALLFORSCHUNG STUTTGART



European White Book on Fundamental Research in Materials Science

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PREFACE

Because we live in a knowledge-based and information-driven society, Europeans are faced with the challenge of globalization. This affects European industry, economy, and academia on many levels. However, the production of new knowledge and know-how is no longer the privilege of only a few nations. We see a world-wide competition to establish and promote the very best centres of excellence in fields where basic insights and the creation of new knowledge produce emerging technologies. In an attempt to gain global leadership, major companies seek to develop close collaborations with these centres across political borders. Unfortunately, in the process they almost completely neglect old and established ties to their respective national academic research systems.

Academic research institutions of the individual European member states have significantly contributed to the present success of advanced technologies and the healthy competitive atmosphere of European Union (EU) industries. However, these institutions and individual centres, which are traditionally supported by national resources, are too small to maintain leadership in the light of the stiff competition from North America, East Asia, and other emerging parts of the world. In the spirit of European cooperation it is therefore absolutely necessary to enhance the creativity and efficiency of the output of research by combining the efforts of the very best research centres of the EU member states, particularly in fields where basic research is expected to create or enhance new opportunities for EU industries. By doing this, we will secure the quality of life in these member states.

To promote industrial growth, a vibrant economy, and social welfare, Europe must be among the world's leaders in all fields of materials science and engineering research. That goal is certainly achievable. Innovations in materials science abound in nearly all arenas of modern European society, including environment, energy, agriculture, health, information and communication, infrastructure and construction, and transportation.

The future promises equally dramatic advances, making materials science a unique and exciting area of great scientific research, with far-reaching industrial, economic, and societal impact. We will see “intelligent” materials that will enable diverse technologies to respond dynamically to changes in the environment. New materials will be synthesized atom by atom. Indeed, the number of possible combinations of atomic assemblies to achieve new structures and properties is seemingly endless, and this mechanistic understanding will provide powerful tools for materials and process development. Quite simply, basic research is the most important research investment a country can make.

The exploitation of these possibilities requires that talented researchers work in multidisciplinary teams that bring together scientists in materials science, physics, chemistry, biology, mathematics, informatics, and engineering. Capital-intensive, large-scale research instrumentation will be required to characterize new materials from their smallest constituents at all scales of assembly to sophisticated equipment for synthesis, processing, and analysis. Computational research and engineering will

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increasingly make use of supercomputers and computer networks. Research in materials science and engineering is capital intensive and its success will depend on international collaboration.

In Europe, the knowledge and expertise in basic materials science is scattered among various research institutions. Thus, the crucial synergistic effect between universities and research institutes of various countries is partly lost and the European materials science potential has not been fully realized. A new European policy is needed for long-term basic materials research. In this respect, the intentions of the European Commission to promote the basic science research landscape in Europe in the next 6th Framework Programme (2002 – 2006) are very refreshing and beneficial to Europe's future economy and social welfare.

The field of materials science has great challenges and is of the utmost importance for Europe; therefore, action is urgent and necessary. It is within this context that the Max Planck Society, Germany's primary basic research organization, has as many as seven different institutes working in materials science and appropriates 13 percent of its total budget for materials science, almost as much as its spends on astronomy and even more than it spends on physics. This demonstrates the importance of materials science within the context of the different disciplines. It also reveals the high expectations of the scientific community and of the supporting political forces for a constant stream of innovation coming from the research on materials.

In this light, the Max Planck Society, together with a large number of leading materials scientists in Europe and in collaboration with the European Commission's Research Area, has taken the initiative to prepare the present European Materials White Book. It is an assessment of basic research in materials science worldwide, highlighting future directions and pinpointing research priorities for Europe. Examples of the societal impact of the field are given, and topics such as materials education, research careers, and the role of the civic scientist are discussed.

It is our firm conviction that the European research centres, if they join forces, are ready to gain world-wide leadership to the benefit of all of Europe.

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EXECUTIVE SUMMARY

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In the year 2000, the Max-Planck-Institut für Metallforschung in Stuttgart, in conjunction with other materials-related institutes of the Max Planck Society, and institutes and universities from all over Europe, decided to prepare a White Book on the topic of "Strategies for Future Areas of Materials Science and Basic Research in Europe." The aims of the studies were:

1. To assess the state of the art and pinpoint future challenges, needs, and research priorities,
2. To highlight the fundamental scientific opportunities in this field,
3. To consider the impact of materials science on society, and vice versa,
4. To find the best ways of attracting more students to the field and ensure high-quality education,
5. To provide guidelines for science policy makers and to offer a basis for fundamental materials science programmes in Europe.

Preparation of this White Book has involved extensive consultation with leading materials scientists, primarily within Europe (most notably from the CNRS in France and the MPG in Germany), but also from the United States and Japan. Discussions were also undertaken with industrial research directors and relevant policy makers.

Materials science can be defined roughly as "the study of substances from which something else is made or can be made; the synthesis, properties, and applications of these substances." This definition covers both natural and synthetic, traditional and advanced materials. For the purposes of this book, however, the discussion is confined to those materials that form the basis of modern, futuristic high technology. These advanced materials include steels and other metallic alloys; superalloys; polymers; carbon materials; optical, electronic, and magnetic materials; superconductors; technical ceramics; composites; and biomaterials. All of these, and others, are discussed in this book in terms of:

1. *Synthesis and processing* to arrange the atoms and larger-scale components of a system into the desired configuration,
2. *Composition and microstructure* to understand the roles they play in determining the behaviour of materials,
3. *Phenomena and properties* to reveal underlying mechanisms,
4. *Performance* to assess suitability for a given application,
5. *Materials design and lifetime prediction* by theoretical and computational methods.

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The Importance of Materials for Modern Technology

Materials science plays a pivotal role in determining and improving economic performance and the quality of life, particularly in the following areas:

Living Environment: Because of pressing environmental concerns more efficient use of material and energy resources is urgently required. Materials science is helping to develop new energy generation technologies, more energy-efficient devices, and easily recyclable, less toxic materials.

Health: Overcoming disease and providing worldwide medical care are high priorities. Materials science, in conjunction with biotechnology, can meet this challenge by, e.g., developing artificial bones and organ implants, safe drug delivery systems, water filtration systems, etc.

Communication: The increasing interconnectedness of our world requires faster and more reliable means of communication. The information and associated computer revolutions closely depend on advances made by scientists working on new electronic, optical, and magnetic materials.

Consumer Goods: Consumers have come to expect global products/services that are delivered rapidly at reasonable prices. Materials science can improve not only the products but also the way they are handled (e.g., packaging), resulting in faster production and delivery times and higher quality goods.

Transport: Whether for business, holidays, or space exploration, materials science is needed to provide durable, high-performance materials that make travelling faster, safer, and more comfortable. Examples are the development of light-weight aluminium bodies for automobiles, brake systems for high-speed trains, quieter aircrafts, and insulation tiles for re-entry spacecrafts.

Challenges for Basic Research in Materials Science

Several challenges face materials science at the beginning of the 21st Century. The first is to convince industry, the public, and politicians of the importance of materials science in driving modern technological development. As there is often a considerable time lag between a scientific discovery and its useful application, people can forget the link that connects fundamental research and future prosperity. Without continued investment in the science base, however, the discoveries of today-and the highly trained experts necessary to develop and exploit them-will not be available for the innovative products of tomorrow.

In the field of materials science, the barriers that divide academia, government institutions, and industry must be reduced if not completely eliminated. Only in this way will it be possible to turn fundamental discoveries into practical applications for the benefit of Europe. Fostering links between researchers, theoreticians, industrial scientists, and managers through collaborative schemes and joint research institutes is an obvious solution, but many important issues can arise. For example, how can we better protect intellectual property rights, and who gets to dictate the research agenda? It is also important that professional advice on such areas as how to attract investment for joint ventures and how to set up spin-off companies to exploit the results of fundamental research be made available to public sector scientists.

Future Directions and Research Priorities

Greater emphasis needs to be placed on the fundamental understanding of materials rather than on applied science and product development. Naturally, application of materials is the ultimate goal, but this needs to be built on a firm theoretical basis so that improvements can be made more efficiently and reliably. Particular attention should be given to understanding a material's behaviour from the atomic/nano-level via microstructure to macrostructure levels using advanced analytical techniques and computer modelling. This strategy applies to both the improvement of conventional "bulk" materials, such as steel, and to new functional materials for increasingly smaller, "smarter" devices. As shown in this report, Europe has the capabilities to provide that fundamental understanding.

Materials by Design

In the past, the search for new and improved materials was characterized mostly by the use of empirical, trial-and-error methods. This picture of materials science has

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been changing as the knowledge and understanding of fundamental processes governing a material's properties and performance (namely, composition, structure, history, and environment) have increased. In a number of cases, it is now possible to predict a material's properties before it has even been manufactured thus greatly reducing the time spent on testing and development.

The objective of modern materials science is to tailor a material (starting with its chemical composition, constituent phases, and microstructure) in order to obtain a desired set of properties suitable for a given application. In the short term, the traditional "empirical" methods for developing new materials will be complemented to a greater degree by theoretical predictions. In some areas, computer simulation is already used by industry to weed out costly or improbable synthesis routes. Greater European collaboration is required to develop computational tool for materials and processing development and for property evaluation in a "virtual" environment.

Nanomaterials

The ability to control, manipulate, and design materials on the nanometre scale (10^{-9} m) will be one of the major technology drivers of the 21st Century. Many research programmes, both in academia and industry, have sprung up around the world over the last few years in an intense effort to harness the potential of these materials for generating new functionalities, minimizing waste and pollution, and optimizing properties and performance. Nanomaterials are being developed from almost every type of material-including polymers, metals, ceramics, composites, and biomaterials. While not confined to any particular materials class or system, nanomaterials, along with the closely associated fields of smart materials and biomimetic materials, are united by the use of a "materials by design" philosophy in their creation. Some of the many assorted applications that are likely to be seen in the future include ultraprecise drug-delivery systems, nanobots for micromanufacturing, nanoelectronics, ultraselective molecular sieves, and nanocomposites for aircraft and other high-performance vehicles.

Smart Materials

One area of research that will revolutionize our concept of synthetic materials, as well as how we interact with our surroundings, are "smart" (or "intelligent") materials. Unlike normal, inert materials, smart materials are designed to respond to external stimuli, adapting to their environment in order to boost performance, extend their useful lifetimes, save energy, or simply adjust conditions to be more comfortable for human beings. Materials will also be developed that are self-replicating, self-repairing, or self-destroying as required, thus reducing waste and increasing efficiency. Smart materials are being developed by combining regular materials from different classes (metals, ceramics, polymers, biomaterials) in complex architectures (e.g., fracture-sensing composites and artificial muscles). Combined with technologies for manufacturing and controlling structures on the atomic scale (nanomaterials) and mimicking biological systems (biomimetics), the possibilities for newer and better materials seem almost endless.

Biomimetic Materials

The rapidly emerging field of biomimetic materials will form one of the most important technologies of the 21st Century. Biomimetic materials seek to replicate or mimic biological processes and materials, both inorganic and organic (e.g., synthetic spider silk, DNA chips, and nanocrystal growth within virus cages). Better understanding of how living organisms produce minerals and composites will open up new areas of research and applications. Materials will be able to be fabricated much more precisely and efficiently, resulting in new functionalities and increased performance (e.g., self-repairing, ultrahard, and ultralight composites for aircraft). To develop these materials, we will need new chemical strategies that combine self-assembly with the ability to form hierarchically structured materials.

Synthesis and Processing

The goal of future synthesis and processing techniques is to allow scientists to construct tailor-made materials from complex arrangements of atoms and molecules with the same precision and control as currently used for manufacturing semiconductors. Promising synthesis techniques described in this report include chemical processing from simple precursor units, soft solution processing, rapid prototyping of ceramic and metallic components using ink-jet technology, microwave sintering, gas-phase methods such as chemical and physical vapour deposition (CVD-PVD) for forming thin films, composite infiltration, and many more.

Computational Materials Science

Computer modelling, using supercomputers, heavy-duty workstations, and personal computers, will be an indispensable tool for basic and applied materials science in the future. It is already an important tool in many areas of science and engineering, including drug design, climate prediction, aeronautics, and even personnel training! Considerable progress has been made over the last 20 years in the simulation of properties and the processing of metals, polymers, and ceramics having increasing complexity. Computational strategies are emerging that pro-

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vide physical and chemical descriptions of materials over larger length and time scales. One of the "hot topics" in computational materials science today is multiscale modelling, which aims to cover several length and time scales with one consistent simulation framework.

Advanced Analytical Techniques

Materials scientists will require new and more powerful analytical techniques so that they can continue the discovery of new phenomena and develop improved materials for the future. Techniques such as high-resolution transmission electron microscopy, scanning probe microscopy, X-ray and neutron diffraction, and various kinds of spectroscopy allow us to examine materials on the atomic level. These techniques need to be developed, improved, and extended further by integrating them with more powerful computers for rapid visualization of data and comparison with computer models. These techniques have an particular importance in the area of materials synthesis, where they can also be used for manipulating and controlling materials on the atomic and nano levels, as in atomic force microscopy.

Materials Science, Society, and Research Infrastructure in Europe

The development of new materials and their applications will eventually affect everyone, not just those in industry, business, or the academic sphere. At this time, when science, technology and society are all rapidly changing, we must not only consider how materials science affects society but also the ways in which society affects the development of materials science.

Social Acceptance of Materials Science

There is a need for an improved public understanding of all forms of science, particularly of a low-profile discipline such as materials science. The materials science community must therefore be more effective in communicating to the public the manifold benefits it brings. Society invests in research not only for the sake of obtaining new knowledge but also to improve human life. Therefore, the public has a right to know what scientists do and how basic science research and achievements affect society. Basic science is viewed sceptically by an increasing number of young people, partly because scientists have failed to convey the relevance and motivation of their research to the nonscientific public.

Strategies for increasing the public's understanding of science include events and programmes designed to expose more high school students to the wonders of science. These can include consultations between materials scientists and high school teachers and authorities on how to incorporate introductory materials science into school curricula; summer internships in industrial laboratories for high school students; and "sabbaticals" for science teachers so that they can take science refresher courses at universities. Other venues for improving materials science's public profile can include TV shows on popular science, research institute/university "open-house" events, and scientific newspaper articles and magazines targeted at the general public that are inspiring and up to date.

Political Support of Science

European governments need to be made aware of the importance of long-term, sustained support for materials science in order to ensure future prosperity and growth for their citizens. Although individual scientific ingenuity and creativity are important, they are no longer sufficient for the groundbreaking research that leads to new discoveries. Large investments in basic research are needed, which requires politicians of vision and leadership.

Other ways that European governments can bring about change in the relationship between the overall population and the scientific community is by (a) creating a favourable climate for investment in basic research, e.g., through tax incentives; (b) opening dialogues between scientists and citizens about scientific issues and the directions European technology should take; and (c) preparing forward-thinking, long-term science policies that give researchers the freedom to pursue curiosity-driven research, with support for turning new discoveries into practical applications. Finally, to ensure that long-term strategies and research programs are founded on sound science, experts in materials science should also be included in joint European Research Councils and their recommendations disseminated to industry, academia, and the general public.

Basic Research and Industry

Both industry and academia are under pressure to focus their efforts on market-related aspects of product/process development at the expense of an understanding of the fundamental science. Many European companies have eliminated corporate or central research laboratories to

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align their R&D efforts more closely with immediate business needs. This is a dangerous policy for the future. Basic research is the most important investment that a company can make, both for its own future and for the future of the society in which it operates. Although "blue skies" research can be costly in the short term, most breakthroughs, although unpredictable, usually result from such research. This report therefore strongly urges all materials-related European industries to increase their investment and commitment to basic research and create flexible research agendas for making the most of new discoveries and research findings.

Pursuing a research agenda in isolation, however, can be an expensive and time-consuming process for an individual company. Companies and academia alike would benefit from improved infrastructure and networks for performing collaborative basic research. Even large pharmaceutical, chemical, and semiconductor companies that have substantial "in-house" research programmes could benefit from European-wide networks because of the extra resources and manpower at their disposal. Materials-related industries are therefore encouraged to establish and take part in cooperative research schemes, particularly the new European Materials Centres described below.

Materials Science and Education in Europe

Europe needs to do a number of things to ensure that there are enough highly trained scientists and talented researchers in the field of materials science.

- A better public perception of materials science and its importance would encourage more young people to choose a career in this field. The wide range of career opportunities in materials science needs to be better publicized in schools and universities. The top European universities should create materials science departments that can attract the brightest students, and that are competitive with the best departments and institutions in the world.

- Despite the current shortage of students studying materials science and choosing careers in this field, the current standards of education and training across Europe are generally high. This level must be maintained or, preferably, improved. Students should be exposed to the latest technological advances and how they are applied in different fields. At the same time, career education must be promoted to inform students about the range of opportunities and career paths available in this materials science.

- Highly trained scientists and talented researchers are needed at all levels of materials research, from industry to academia. Better incentives are needed to ensure that European researchers continue to work in Europe rather than moving abroad, and obstacles to non-European researchers working in Europe need to be removed. A growing number of materials science graduates are turning to careers in other fields. Therefore, steps should be taken to ensure that none leave because of poor career opportunities or lack of financial rewards. The number of women studying materials science also needs to be increased, and greater support provided for career progression.

- The ideal balance between basic and applied research needs to be found to ensure Europe's long-term prosperity. The establishment of dedicated European Centres of Competence in Materials Science and Technology that will undertake fundamental research on behalf of industry, but are also connected to universities, is one way to make the most of Europe's scientific potential.

  - Long-term fundamental research should be pursued at *European Centres for Materials Science*, and also encouraged at universities, with researchers benefiting in terms of ideas and training from contact with industry.
  - Short-term research programs with industrial relevance can be carried out at the *European Centres for Materials Technology*, with input from university and industrial researchers in a collaborative framework.
  - Long-term industrial research (to meet particular strategic needs) should be undertaken within the partner company, with the short-term research centre projects serving as feasibility studies.

- Modern materials science is an increasingly interdisciplinary activity in which physicists, chemists, biologists, mathematicians, computer scientists, and engineers can all contribute their expertise to a wide range of scientific and technical problems. The growing fields of nanotechnology, biomaterials, biomimetic materials, and smart materials will not prosper without intensive crossover and interaction between disciplines. Fresh ideas, new insights, and innovations will undoubtedly result from greater multidisciplinary interaction. To reap the rewards of an interdisciplinary approach, universities and research institutes need to encourage more flexible movement between disciplines by (a) breaking down rigid administrative structures and (b) setting up multidisciplinary groups or centres. National governments, funding agencies, and the EC should also encourage interdisciplinary activities by:

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- Sponsoring regular workshops, conferences, and summer schools that focus on multidisciplinary areas in materials science
- Supporting the establishment of cross-disciplinary research programmes
- Encouraging agreements between funding agencies for the establishment and coordination of multidisciplinary materials research, e.g., bio- and medical materials
- Granting fellowships and other financial support to scientists moving from one field to another

Major Research Facilities

Equipments – necessary for many important characterization methods – are becoming increasingly sophisticated and are often too expensive for single medium-sized companies or university departments to afford. Therefore, a strong component of the EC's basic research support should be equipping and supporting large multiuser facilities at specific locations. In the case of materials science, these facilities should include the latest high-energy electron microscopes and synchrotron and neutron radiation sources (e.g., to examine crystal structures and chemical bonding), high-pressure anvils, and supercomputers. They will also serve as a place of contact between experimentalists and theoreticians, and researchers from different disciplines. In addition, these state-of-the-art facilities will attract the world's leading scientists, helping Europe to maintain the highest levels of scientific excellence.

European Centres for Materials Science and Technology

European Centres of Competence in Materials Science and Technology need to be established to foster cross-fertilization of ideas and state-of-the-art science. They should include a basic research programme that gives graduate and postdoctoral students the opportunity to perform world-class experiments. The centres should also organize workshops, short courses, summer schools, industrial visits, educational programmes, etc., for training scientists and engineers. These could be newly established "brick-and- mortar" centres, "virtual" (i.e., networked) centres, or extensions of current European materials research institutes. The best of them could be designated "Materials Centres of Excellence," with extra funding and higher wages earmarked for these institutes so as to attract the best and brightest from around the world. This strategy will help motivate European researchers to return to Europe after stints of working abroad.

European Research Networks

Materials science has advanced to the point where it is often impractical (or indeed impossible!) to assemble in one place all of the intellectual resources and speciality equipment needed for a large-scale project. "Virtual" centres, or networks for materials science will be formed of research laboratories from academia, industry, and major facilities. These centres will be linked by high-speed Internet connections and will act as hubs for interdisciplinary research. This will be the most efficient use of the research infrastructure and facilities that are spread throughout different Member States.

General Recommendations

This study has identified four major themes that can serve as a guideline in discussing the advancement of materials science research in Europe:

1. The importance of materials science to the prosperity of future Europeans, and indeed, humankind
2. The need for better theoretical understanding of materials and their behaviour, and the fundamental research needed to obtain this
3. The highly interdisciplinary nature of materials science, and the excitement and personal rewards that a career in this field can bring
4. The need for continued, long-term investment, particularly basic research, by national governments, industry, and the European Commission

The relevance of materials science to modern society needs to be emphasized and promoted beyond the research community and industry to governments and the general public. Forward-thinking and sustainable initiatives for materials science research need to be launched that will attract the world's best scientists and ensure that more fundamental discoveries come our way during the next century. With the cooperation of government, industry, academia, and the general public, European materials science research can remain at the forefront of developments. We hope that this report will aid the discussion of how this can best be achieved.

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INTRODUCTION

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Humankind's existence has always depended on the availability of materials. Indeed, historians use the dominant materials of an ancient era to classify it: they speak of the Stone Age, the Bronze Age, the Iron Age. This reliance on materials has continued to the present day, not only for our physical existence – clothing, buildings, transport, and the innumerable other inventions that have marked human progress – but also for our cultural and intellectual lives as well-literature, art, music. In fact, without materials the human endeavour would hardly be conceivable.

The latter half of the 20st Century was characterized by profound improvements in our knowledge and ability to create new materials to a degree that could only be dreamed of a hundred years ago. These advanced materials underpin all modern technologies, from silicon chips to jet engines to medical imaging. Because of this increased use of and reliance on new materials, society needs to refocus its emphasis on materials development, something that it has often neglected in the past. This requires a re-evaluation of the role of materials science in society in order to guarantee the availability of new tools with which to solve some of the most pressing problems the world faces today, such as environmental pollution, a dwindling supply of resources, overpopulation, and disease epidemics.

The growing public awareness of these issues coincides with the intention of the European Commission (EC) to reshape the fundamental research landscape in Europe. This has resulted in closer links between the EC and the Max-Planck-Institutes involved in materials science and inspired the idea of compiling this White Book on "Fundamental Research in Materials Science."

Work on the project began with a discussion meeting between June 13 and 15, 2000 at Ludwigsburg, near Stuttgart, Germany, in line with the preparation of the new EC 6th Framework Programme (2002 – 2006). About 75 leading scientists from Europe and the U.S., including experts in the disciplines of materials, mathematics, physics, chemistry, biology, information technology, and engineering, met for two days of brainstorming about the many different aspects of materials science. (The programme is provided in Appendix I and the list of participants in Appendix II).

Topics were selected and reviewed. For each topic, acknowledged experts introduced the state of the art and presented their visions for future evolutionary developments and revolutionary breakthroughs. This was followed by open discussions with scientists in the audience.

After the workshop, teams were formed and team coordinators appointed. Each coordinator and team provided a written summary of their discussions and ideas. Emphasis was placed on the directions and opportunities for future materials research, with reference to the social and economic implications where relevant. This input formed the basis of this White Book.

The initial conclusions, recommendations, and future research opportunities resulting from this exercise were discussed further at a second workshop on March 15/16, 2001 in Degerloch, again near Stuttgart. (The programme is provided in Appendix III and the list of participants in Appendix IV). Attendance at this meeting was limited to the coordinators, policy makers, representatives of the EC Director-General for Research, heads of national laboratories, and industrialists.

Throughout this period, close contact was maintained with the EC Research Directorate for Materials to coordinate our efforts to resulting in new research initiatives.

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The format of the White Book follows the format of this second meeting. That is, a wide variety of different classes of materials and techniques are examined from as many viewpoints as possible. Contributions from many different authors, all respected and acknowledged experts in their fields, are grouped under the following chapter titles: (1) Materials: Science and Engineering; (2) Materials: Science and Applications; (3) Interdiscipinarity in Materials Science; (4) Materials Modelling and Materials Theory; (5) Materials Phenomena; (6) Materials Synthesis and Processing; and (7) Advanced Analytical Techniques. Individual scientists or teams of scientists wrote the individual chapters of each section. The author(s) bear(s) full responsibility for the content of their chapter. (A list of authors is provided in Appendix V). A few topics were discussed and analyzed by different scientists from different points of view. This has led to a slight overlap of a few topics.

It should be emphasized that the White Book does not claim to cover all areas of materials science in detail. The chosen subjects reflect the view of the individual scientists present. Nevertheless, we believe that we have covered the main topics relevant for the broader development of materials science.

The White Book sheds light on recent advances in fundamental research in each of these materials-related fields. It highlights the great importance for new synthesis and characterization methods, the search for new phenomena and materials, and the growing use of computer models and theoretical understanding in all areas of materials science. One of the major theme, which came through clearly and consistently from both, the meetings and the articles contained in this book, is that the future of materials science lies in the crossover and exchange of ideas between disciplines. Consequently, a special chapter (Chapter 3) has been devoted to the interdisciplinary nature of materials science and how best to foster it. This interdisciplinary aspect must also include engineering. Because fundamental research in materials science eventually results in a product that serves society, materials – both traditional and advanced – must be "engineered" at all length scales. Engineering at the smallest length scale results in "nanomaterials" which open up new research horizons; not only for tailoring complex materials with specific and superior properties, but also for exploring new phenomena that arise when matter is confined to within molecular-sized structures.

An expansion of interdisciplinary research would be to consider materials science, including fundamental research, as a holistic concept ranging from processing to recycling of materials – each step emphasizing also ecological aspects. The holistic approach of materials science is essential for the future welfare of society.

Chapter 8 examines the social aspects of science, including new schemes for materials education, careers for research scientists, and inter-European and international mobility of researchers. In addition, a new strategy for basic materials science research in Europe is presented, with suggestions on how to organize European research efforts to the best effect.

The overall conclusions, recommendations, and directions for future research are summarized in the final chapter (Chapter 9), which highlights the importance of basic materials research to economic growth and prosperity. This chapter also provides insights into the research needs of various materials classes and gives directions for future research opportunities and activities in the materials science area.

The book as a whole is oriented towards fundamental aspects of materials research, but visions of the future and other opinions from industrial research authorities were also taken into consideration. An important example of this is the role that basic materials research will play in future European transportation systems. Materials science also has an important part to play in alleviating many of the environmental problems that we now face, not least of all by developing new energy-efficient devices using fast ionic conductors and improved catalysts.

The audience for this book, therefore, is large. It is addressed to all materials scientists and scientists from materials-related disciplines in Europe, as well as national and European policy makers. Because of the necessity to focus on materials development, this book is also of important to industry, especially small and medium-sized enterprises. As well as providing an up-to-date account of the latest technology and research topics, it also provides ideas for future innovations, devices, and applications of materials. If these can be developed by European industries, then Europe's economic prospects, and consequently its citizens' welfare, will be much the better for it.

This book serves as a call to European politicians to upgrade their investment in basic materials science at least to a level comparable with that in other industrialized countries, notably the U.S. and Japan, so that European industry can remain competitive well into the future, and we can pass on a culturally, scientifically, and economically flourishing Europe to future generations.

The editors of the White Book thank all the authors, helpers, workshop participants, and colleagues from all participating Max-Planck-Institutes, and The Max Planck Society, for the enormous effort they have put in to making the publication of this book possible. The support by Dr. Stephan Krämer, MPI für Metallforschung Stuttgart, during the editing and printing of the White Book is greatly acknowledged.

We trust that this White Book will result in the reinvigoration of materials science in Europe. We especially hope it will open the eyes of the public, opinion makers, and politicians to the wonders of materials science, the benefits it brings, and its role as one of the main pillars of economic progress and social well-being in Europe and, indeed, the world as a whole.

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1. Materials: Science and Engineering

Introduction

Materials science is an interdisciplinary research area which covers the physics, chemistry and engineering of all classes of materials. Traditionally, these materials are divided into metals and metallic alloys, ceramics, semiconductors and other inorganic materials, and polymers and organic materials. Recently, the science of materials has received increased attention because of the discovery of new classes of materials and their application in new technologies.

The traditional classification of materials into different classes or types is still helpful since specific engineering applications still rely on components made from materials from one or other of these groups. In this chapter it will be shown that metals and metallic alloys (including composites) still constitute the majority of structural and functional materials used within the EU, as well as worldwide. Use of this group of materials has an enormous technological and ecological impact on society, and one of the challenges of materials science is to come up with metals with improved properties via cheaper processing routes. This is especially true for the automotive industry where synthesis and processing controls the microstructure, properties, and performance of metallic materials. It is now well appreciated that for this industry-which consumes enormous amounts of metals-to be sustainable, automobile design must encompass the complete lifecycle of the materials used, from processing to recycling.

◀ Microstructure of polytype SiAlON (transmission optical micrograph obtained with polarized illumination, U. Täffner, MPI für Metallforschung Stuttgart).

The distinction between ceramics and other non-metallic inorganic materials is often difficult to define. In this chapter two aspects of these materials are described, namely fundamental research and real-world applications. The future of non-metallic materials appears to lie in development and exploitation of specific functional properties. As a group, ceramic materials have perhaps the largest range of functions of all known materials, and can be used for a diversity of applications. It is very important to understand the fundamental processes which lead to specific properties. In simple terms, ceramics are compounds or mixtures of compounds of metallic or metalloid elements with non-metal elements.

The properties of a particular material depend not only on the chemical nature of its atoms, but also on their arrangement and distribution in its microstructure (grains, pores, etc). Materials with specific thermal, mechanical, nuclear, electrical, magnetic and optical properties can be fabricated. Due to the staggering variety of these materials and their possible combinations, there is still a huge amount of research that needs to be done. So far only a fraction of the inorganic materials that could possibly be put to use have been studied, and there is little doubt that many new compounds with unusual or superior properties are still to be found.

Inorganic solid state chemistry and physics investigate the basic principles and provide the necessary background for research into the correlation between microstructure and properties of inorganic compounds. Insights can been gained simply by comparing phenomena of different ma-

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terials with each other, but more rigorous understanding based on quantum theory is also necessary for today's advanced materials.

Polymers find increasing number of applications every year. Recently, however, research into "traditional" polymers has declined. At present the polymer manufacturing industry in Europe is undergoing major restructuring, which has led to severe cutbacks in companies' Research & Development (R&D). To fill this gap, universities should increase the amount of fundamental research they do into polymeric materials.

All life-forms are based on soft organic materials; polymer science can therefore also be related to our understanding of biological materials, particularly carbon-based materials. Ceramics, on the other hand, are similar to hard biological materials such as teeth and bone, so that connections between these two fields will continue to grow as well. We can expect many more functionally useful materials to become available in the future by manipulating the chemistry and processing techniques of all these materials, and combining them in new ways.

Carbon materials have received a lot of attention recently through specific modifications such as graphite sheets (rolled up to form nanotubes or buckyballs) and synthetic diamond. The basic principles of inorganic carbon chemistry are understood. These specific forms of carbon are expected to be useful for a variety of applications in different branches of engineering. Hence it is very important that links between the science of carbon and its applications be strengthened.

It is difficult to imagine modern society functioning today without electronics. Electronic, optical, and photonic materials play essential roles in information technology, computing, and systems control, as well as electronic consumer goods. There is a great deal of commercial pressure to develop new materials for use in these areas. Fundamental research into electronic, photonic and optical materials is therefore essential for the continued improvement and miniaturization of electronic and photonic devices.

The following eleven sections summarise the state of the art for the different classes of materials. Expected evolutionary and revolutionary developments are sketched in each section.

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1.1. Metals and Composites: Basis for Growth, Safety, and Ecology

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1.1.1. The Place of Metals in the World of Materials

Metallic alloys and composites represent the dominant group of structural and functional materials world wide and within the EU. This applies for their technological impact on society as well as for the scientific challenges associated with further discoveries and developments in this field. Fundamental and long-term oriented research on metals and composites leads to the development of well-tailored technological solutions which serve society with respect to sustainable progress, ecological benefits, advanced safety demands, and economic success. Prominent challenges along these lines lie in understanding and developing the fundamentals of lightweight structural materials and design solutions, self-organising microstructures, failure-tolerant materials systems, smart materials, and materials for ground and aerospace transportation (Fig. 1.1 and 1.2).

This report gives an overview of the most important future research topics in the field of metals and composites research as collected and discussed within a group of about 100 leading experts from the EU, Asia, and the U.S. It gives corresponding recommendations for future basic research initiatives on metallic alloys and composites in the 6th EC Framework Programme.

1.1.2. State of the Art and Expected Trends

The state of the art in the field of metals and composites research is characterized by a mature level of property optimization and characterization particularly as far as bulk mechanical aspects of conventional structural metallic materials are concerned. Basic principles behind bulk materials kinetics and thermodynamics in such alloys are understood to an extent that they can be used for the further gradual optimization of existing alloy concepts with respect to structural and/or functional properties. Recent European programmes have focussed on improving and tailoring existing material concepts for matching technological and commercial boundary conditions and on designing new materials concepts beyond conventional R&D lines.

This research concept of the past decade has for many aspects matured to a level where future activities, when

Fig. 1.1. Space vehicles which are at the cutting edge of high technology are built of structural elements of steels, aluminium, magnesium and beryllium alloys and metal-matrix composites.

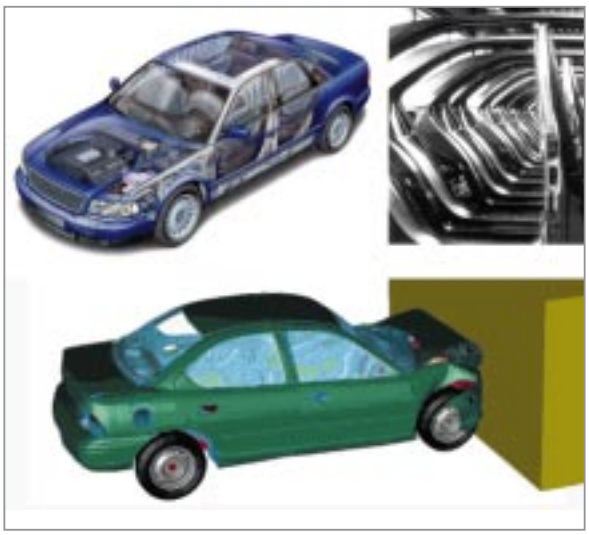

Fig. 1.2. Modern automotive technology relies on safety equipment made of advanced steels, aluminium, and magnesium alloys.

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designed and pursued along the same lines as before, will lead to a more and more asymptotic research progress. Future long term research programmes must, therefore, formulate concepts to achieve distinct progress steps leading EC projects beyond existing research plateaus. This approach would maintain and strengthen the position of metals and composite research as a key science and technology providing progress-critical input to other key areas of science and high technology. It should thus be the aim of future research in this field that coming technology applications are being pushed forward by materials rather then vice versa.

Some key rules can be formulated to unleash unused potential of metallic and composite materials through a new European framework research initiative with the aim of entailing fundamental progress steps pushing this discipline beyond existing R&D asymptotes.

• First, EC projects should make extensive use of *novel experimental and theoretical tools* as well as advanced combinations of them. Although further improvements and applications of well developed "workhorse" methods are essential to provide serious and systematic data for novel materials concepts, it is less likely that they play a bottleneck role in future metals research such as the use of novel methods which will allow new observations, which have not been made so far (some of the new research tools will be specified below).

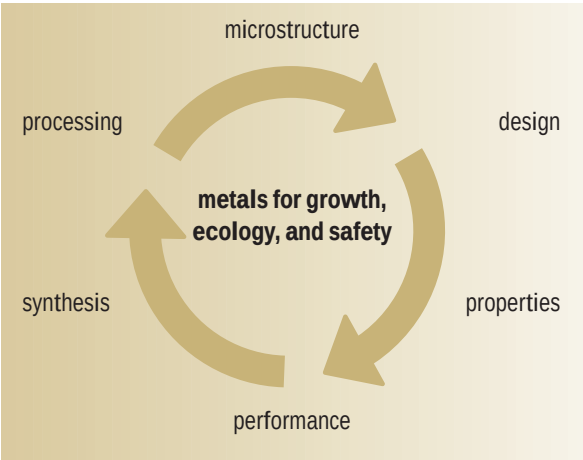

Fig. 1.3. Essential elements of advanced metals and composites research.

• Second, EC projects should address *fundamental long-term problems of existing and cutting-edge structural and functional metallic materials concepts* which are the basis of our economy but are not covered by applied or industry research. In this context it is important to note that industry pushes materials developments only to a level of immediate commercial output and leaves behind numerous unanswered questions which often affect ecological, economic, performance, and safety aspects. Such concepts deserve in part more attention from the fundamental side in order to avoid long-term misconceptions and exploit and development better the potential of existing materials.

• Third, EC projects should create *materials concepts far beyond conventional approaches*, focussing particularly on so far less exploited combinations of different material classes, property-structure integrations, and property profiles. In this context it is important that new materials development should be accompanied from the beginning by fundamental research since material development is nowadays an integrated and interdisciplinary task.

• Fourth, future research initiatives should give very high priority to projects with highly *interdisciplinary character* closely integrating concepts and approaches from areas such as materials physics, materials engineering, information technology, materials chemistry, mathematics, and/or biology.

1.1.3. Outline and Principles of Future Research Strategy

The basic research strategy required in this field can be classified into two major disciplines. The first one comprises *experiments on model systems*. The second one comprises modelling and computer simulation. As far as metals and composites are concerned the latter branch particularly concentrates on macro- and mesoscale simulation issues.

Experiments on model systems should map essential ingredients of composition, synthesis, processing, and microstructure design which are not well understood but have key functions in novel material design as well as advanced conventional materials concepts (Fig. 1.3). The following key points might characterize projects in this field:

• First, projects should make use of *novel experimental tools and/or advanced combinations of experimental tools* exploiting observation methods that have not yet matured to their full potential. Examples (see section 1.1.4) are nano-mechanical property characterization in conjunction with nanoscopic analytical and orientation characterization; 3D atom probe methods; high-resolution analytical microscopy in conjunction with automated high-resolution orientation imaging microscopy; 3D synchrotron X-ray microscopy; field ion beam microscopy in conjunction with high-resolution orientation imaging microscopy in

FEG (FEG = field emission gun) scanning electron microscopy; advanced neutron scattering methods; *in situ* experimentation combining sample observation with heating or mechanical loading. Consideration must also be placed on fast and appropriate analysis tools which are capable of extracting and visualizing relevant information from the ever increasing experimental data sets.

• Second, projects should address *fundamental long-term problems of existing structural and functional metallic materials concepts* by use of model experiments which are the basis of our economy but are not covered by applied or industry research. Examples are integrated model design solutions exploiting materials as well as constructional aspects; metal-metal interfaces and grain boundary triple-points in the form of well-defined model bi- and tricrystals; metal-metal joints; advanced structural-functional as well as smart compounds.

• Third, projects should create experimental *model systems heading beyond conventional approaches*, focussing particularly on so far less investigated combinations of different material classes, microstructures, and property profiles. Examples are entangled, cellular and porous metallic microstructures; nanoscale metal-polymer compounds; ultra thin layered metal-ceramic-polymer structures; nanostructured functional-structural composites; woven metallic systems; nanoscale integration of metals, polymers, and ceramics; self organising metal-polymer interfaces; composite foams; and metal-semiconductor-polymer sheet compounds.

• Fourth, design of model systems should be particularly pursued in projects with highly *interdisciplinary character* closely integrating concepts and approaches from materials physics, materials engineering, materials chemistry, mathematics, information technology, and/or biology. Examples are the application of nanoscale materials mechanics tests to large sets of material samples or graded samples using variational alloy chemistry methods in conjunction with nano-indentation; the design and investigation of metal-polymer interfaces with high-resolution analytical experimental tools as projects between metal physics, physical chemistry, and process engineering; determination of elastic and plastic response of ultra thin layered structures under thermal, electromagnetic, mechanical loadings, or environmental loadings as projects between metal physics, physical chemistry; process engineering; design and investigation of self organization effects in metal-polymer and metal-ceramic interfaces as projects between ceramics, metal physics, physical chemistry, and biology; and closer cooperation between experts from theory and experimentation.

Modelling and computer simulation projects should aim at a fundamental understanding and a prediction of the performance of novel and advanced conventional structural and functional materials. The recognition of these basic needs from the theoretical side, along with the ever increasing computing power, has established computer modelling approaches as one of the major areas in materials research. In this approach one formulates model descriptions based on fundamental principles and investigates their properties and behaviour by numerical simulations. Modelling and computer simulation will play a key role in understanding, tailoring, and predicting materials synthesis, processing, microstructures, and properties. While modelling can produce realistic results for very complex situations, underlying theories, based on results of modelling, must be built as history-dependent and multi-scale concepts, integrating electronic and atomic level as well as continuum scale information whenever relevant (Fig. 1.4). These allow generalization and deep physical understanding of phenomena studied. Modelling and simulation tools have in recent years matured to a state where available software is increasingly well designed and maintained and built on robust theoretical and mathematical grounds.

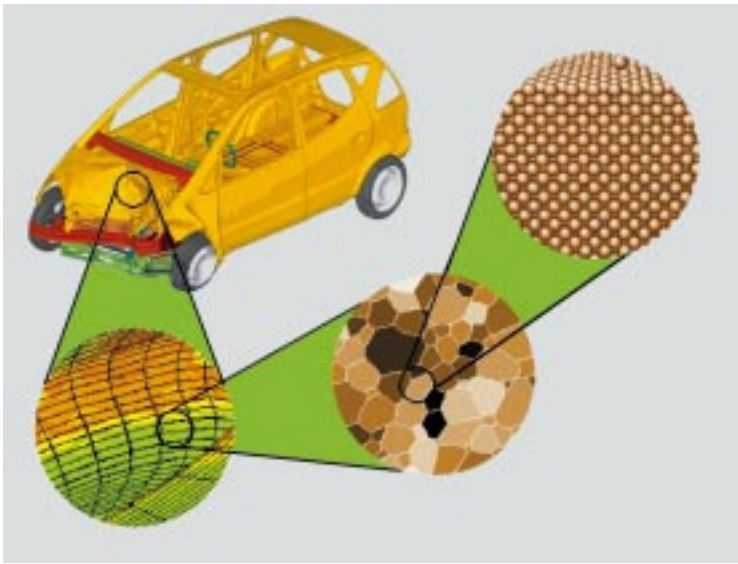

Fig. 1.4. Important hierarchical scales of computer simulation methods in the field of metals and composites research. Future developments must integrate macroscopic finite element predictions, mesoscale methods, and atomic scale simulations for the design and optimization of new advanced products.

Distinct progress steps pushing this field of computer simulation forward can only be expected when the above mentioned key points are considered. This means that

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• First, projects should make use of and better integrate novel tools from *theory, mathematics, and information technology*. Examples are better exploitation of parallel algorithms and parallel computing power; application of distributed computing based on high speed network connections; development of robust and fast parallel non-linear variational methods for tackling large quantities of coupled differential equations; critical reliability investigations of numerical methods and existing codes; standardization and sharing of computer codes and resources; closer integration of electronic ground state and atomic scale calculations into continuum concepts; improvement of physically motivated strain gradient and crystal plasticity continuum theory; better integration of and comparison with experimental data in case of non *ab initio* methods; development of fast though robust simulation algorithms for the electronic, atomic, and continuum scale; and direct coupling of electronic and atomic dynamics simulations beyond the Born-Oppenheimer approximation. Furthermore, particularly large scale simulation efforts require closer integration of materials and constructional/ design issues. For instance, aspects such as the overall part stiffness results from ingredients of both areas. Such projects should introduce design-oriented database-related approaches exploiting artificial intelligence methods. Another important point of integration are joint simulations of functional – constructional devices. Also, one should draw more attention to novel information treatment methods such as the neural net and fuzzy logic approaches.

• Second, simulations should aim at structure- and property predictions of model systems pertaining to *existing structural and functional metallic materials.* Focus should be placed on the mesoscopic and macroscopic scale. Examples are anisotropic continuum scale CPFE-based simulations (CPFE = crystal plasticity finite element methods) of elastic-plastic co-deformation of metallic systems as well as corresponding simulations considering metal-polymer and metal-ceramic compounds; micromechanics predictions of polycrystalline matter under mechanical loads; micromechanics predictions of woven and foam composites; joint microstructure simulations integrating casting, thermomechanical and cold forming issues; and GL-based simulations (GL = Ginzburg – Landau – type phase field methods) of structure- and concentration-dependent topological mesoscale aspects.

• Third, simulations should aim at designing and predicting structure- and properties of *novel material concepts* at the electronic-, atomic-, meso-, and macroscale. Examples are LDF-type electronic scale predictions (LDF = local density functional theory) of the influence of foreign atoms on metal-metal interfaces; MD-based simulation (MD = molecular dynamics) of interfaces and crack tips under loads; CPFE-based continuum scale simulations of behaviour under elastic-plastic loads; GL-based simulations of metal-polymer, metal-semiconductor, and metal-ceramic compounds; mesoscale joint GL- and CPFE-based predictions of self organization kinetics at metal-polymer interfaces; micromechanics predictions for woven and foam composites; atomic scale process design simulations for micro- and nanoscale compound tailoring using hyperdynamics concepts.

• Fourth, simulation projects should be particularly pursued in projects with highly *interdisciplinary character* closely integrating concepts and approaches from materials physics, materials engineering, materials chemistry, mathematics, information technology, and/or biology. Examples are the integration of electronic ground state simulation into continuum models as projects between physics and materials science; integration of polymer mechanics and metal mechanics into predictions of layered structures as projects between materials mechanics and physical chemistry; development of faster simulation methods and algorithms as projects between mathematics, information technology, metal physics, and chemistry; the development of parallel and distributed methods as projects between mathematics, information technology, metal physics, and chemistry; and closer cooperation between experts from theory and experimentation.

1.1.4. Details of Future Research Programme

(a) Introduction

Based on the concept explained in Sect. 1.1.2 this part gives a more detailed outline of recommendations for future research topics in the fields of metallic alloys and composites. The organization of topics in this chapter follows in the first place the key subjects as agreed at the Ludwigsburg symposium but gives suggestions with relation to the above introduced organization of projects into model system experimentation and computer simulation. The key areas of future fundamental research in the field of metallic alloys and composites as agreed at the Ludwigsburg symposium are:

- Interface science and microstructure design
- Thermodynamics and kinetics
- Synthesis and processing
- Mechanical and functional properties

(b) Interface science and microstructure design

Laws of interface motion and energy often follow strong dependencies on state variables. Metal and composite

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interfaces typically have bottleneck function in materials properties and design. It is likely that substantial new fundamental insights and outstanding progress in performance can be expected particularly from metallic alloys and composites with a high density of homophase and heterophase interfaces. Such concepts can be realized in the form of bulk systems with intricate 3D interface percolation, layered systems, and bamboo-type structures.

The key focus in this area is a better understanding of nucleation events and the role of the mechanisms of interface formation as well as interface motion. Materials are getting increasingly dominated by interfaces. This includes metal / ceramic, metal / metal, metal / polymer etc. interfaces. Investigating such phenomena requires to focus on the electronic and atomic aspects as well as on macroscopic aspects.

Topics in this context with fundamental importance include:

1. self-organising and self-repairing surfaces and interfaces
2. generation, structure, and properties of interfaces with fractal dimension
3. nano- and microtribology
4. interface and surface systems under thermal, elasto-plastic, electromagnetic, environmental and coupled loadings
5. surface- and strain-driven continuous and discontinuous subgrain coarsening
6. elastic-plastic and functional interaction across heterophase and homophase interfaces
7. nucleation phenomena
8. mechanics at interfaces
9. interfaces and surfaces turbine blade alloys under complex loadings
10. functional/structural optimization of interfaces
11. interface phenomena in woven and foamed metals and composites including corrosion
12. role of interfaces in smart materials, particularly in nanoscale filter, electronic, and catalytic matter
13. interface mobility and effects of other lattice defects, triple junction effects
14. recrystallization and grain growth phenomena
15. orientation and misorientation evolution at the nano- and microscale
16. grain cluster-mechanics
17. micromechanics of interfaces and surfaces
18. precipitation phenomena under complex loadings, in constrained and layered systems, and in multi-component systems
19. interface design and manipulation

(c) Thermodynamics and kinetics

Thermodynamics and kinetics data are essential for tailoring and predicting novel materials. Particularly in interface dominated systems thermodynamics and kinetics are not well understood though they have key function in novel materials design. Topics in this context with fundamental importance include:

1. thermodynamic and kinetic data of multi-component systems and interface-intensive systems
2. transformations under elasto-plastic and electromagnetic loads, effects of point and line defects on interface transformations
3. transformation in confined, low-dimensional, layered, and small scale structures
4. development, standardization, and intercalibration in the field of experimental materials thermodynamics
5. Non isothermal and reversal problems in heat treatment
6. microstructures arising from competing kinetics

(d) Synthesis and processing

Microstructure design will play a critical role in the synthesis of novel multi-layered and small scale structured materials. Key points to be addressed are the fundamentals of:

1. self-organization and self-assembly of microstructures with desired properties
2. *in situ* processing of functional-structural materials
3. layered and graded structures
4. super strong metals composites, matter close to the limits of theoretical strength
5. ordering effects of magnetic particles and domains
6. metallic foams
7. casting defects
8. microstructures inheritance in materials processing
9. nanoscale particles: processing, self organization, quantum dots
10. fabrication of bulk and thin film nanostructured metals
11. microstructure percolation effects
12. intermetallics and oxides: combination of high strength, ductility, and creep/fatigue resistance, internal oxidation
13. *in situ* nanostructuring through deformation, metallurgical methods, deposition, and diffusion
14. *in situ* decomposition
15. field assisted annealing
16. high temperature alloys and compounds: turbine materials, aerospace composites, alloys for hot and aggressive environment
17. joining processes

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(e) Mechanical and functional properties

A strong overlap should be created between interface and plasticity projects. In the field of plasticity the following areas of fundamental interest were identified:

1. collective behaviour of structural defects
2. scale-bridging plasticity and failure concepts in materials simulation and experiment
3. elasticity and plasticity in confined, layered, graded, and nanoscaled materials
4. effects of solute elements on work hardening
5. anisotropic elasto-plasticity of polycrystalline matter
6. internal stresses in conjunction with plasticity and transformation
7. void nucleation and coalescence
8. mechanics of entangled and percolated systems: metal wool, cellular solids, dendritic structures, scale and gradient effects in plasticity
9. textures at the micro- and nanoscale: coupled stress and texture determination
10. interaction between environment and plasticity
11. high strength - high conducting composites
12. grain cluster mechanics
13. mechanical, transformation, and precipitation fundamentals of novel lightweight Mg, Be, Al, Fe alloys and intermetallic-based lightweight alloys under complex loadings
14. mechanical properties of alloys and intermetallics doped with rare earth elements
15. integrated structure and materials optimization: integrating design and materials properties
16. mechanical-functional materials properties as inverse problems, i.e. back-extrapolation of optimum thermodynamics and microstructures from desired final properties.

1.2. Advanced Ceramic Materials: Basic Research Viewpoint

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1.2.1. Introduction

Ceramics are a class of materials broadly defined as “inorganic, nonmetallic solids”. They have the largest range of functions of all known materials. Despite the already existing variety of compounds, the number of processing techniques, and the known diversity of properties and applications of the materials, all advanced countries share the need for basic research in several areas: finding *new compounds with improved specific properties*, increasing knowledge of *fabrication processes* for economical and ecological ceramic parts production, *miniaturization and integration of ceramics with similar or dissimilar materials*, and building a better understanding of materials behaviour through *computational modelling*.

1.2.2. State of the Art

The last decades have seen the development of the enormous potential of functional ceramics based on unique dielectric, ferroelectric, piezoelectric, pyroelectric, ferromagnetic, magnetoresistive, ionical, electronical, superconducting, electrooptical, and gas-sensing properties. Such properties now constitute the basis of a broad field of applications (Fig. 1.5). Scientific advances concerning many ceramic materials have enabled technological breakthroughs of truly global proportions.

Similar scientific developments also have taken place in structural ceramics. Thermal, chemical, and mechanical stability of many oxide and nonoxide compounds laid the foundation for improved processing, which led to an improved level of microstructure design and defect control. This in turn resulted in never-before-seen improvements in mechanical performance and in the reliability of the properties of components and devices.

In addition, superior combinations of thermal, insulating, and mechanical properties have become the basis of huge applications in the packaging of microelectronics and

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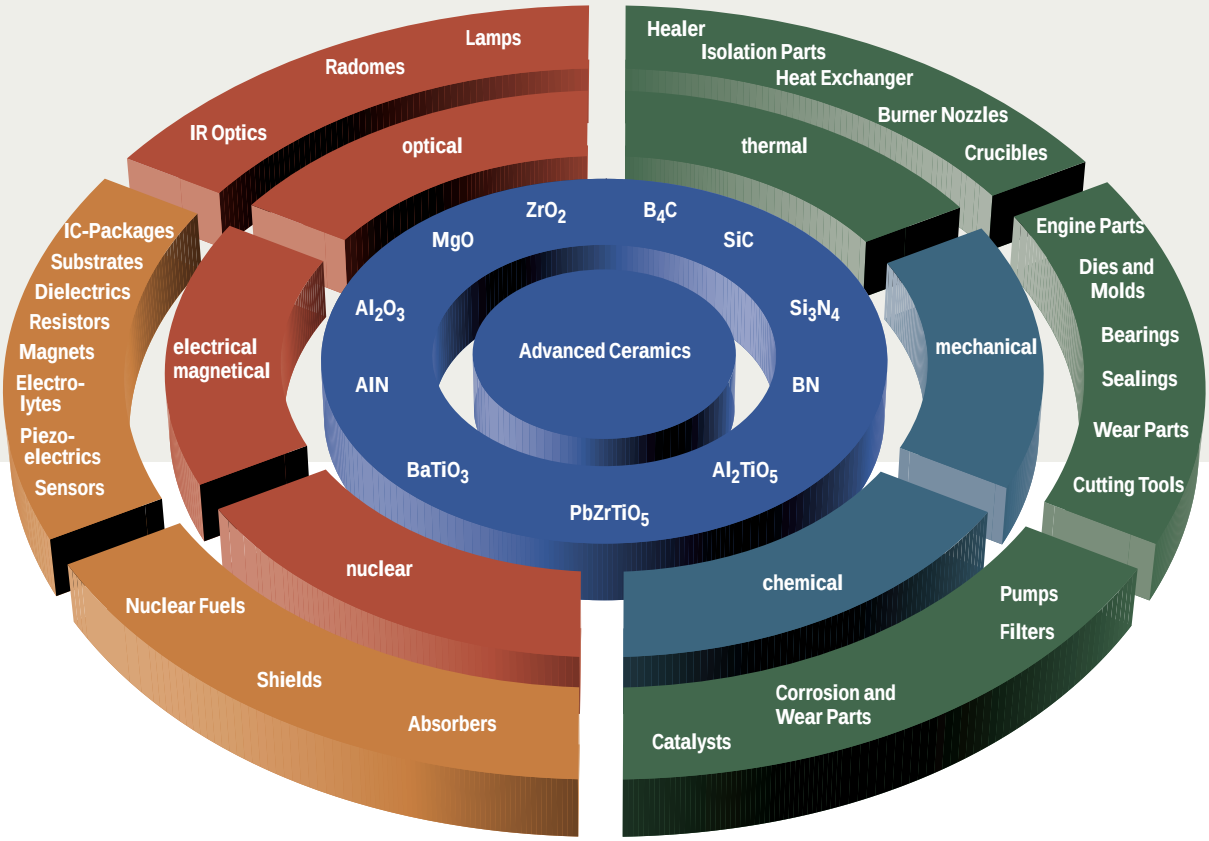

Fig. 1.5. Functional and structural applications of advanced ceramics.

power semiconductors. Therefore, ceramic materials have now become the cornerstone of such advanced technologies as energy transformation, storage and supply, information technology, transportation systems, medical technology, and manufacturing technology (Fig. 1.6).

Since technical and economical progress in such areas is in line with the mastering of materials, empirical fabrication procedures are progressively being replaced by knowledge-based production and engineering. Therefore, today's advanced materials synthesis and processing, and the economical manufacturing of components and devices are being driven more and more by an increased understanding of the underlying fundamental scientific phenomena.

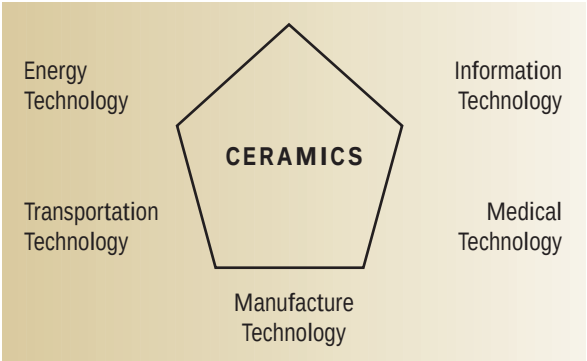

Fig. 1.6. Technology areas which benefit from advanced ceramics.

1.2.3. Trends in Technology

Since production and engineering of materials and components are increasingly knowledge-based, the technology itself reveals gaps in the basic understanding of materials. Such gaps limit the degree to which materials technology can be competitive with other technologies. Therefore, the continued pursuit of additional knowledge will always be necessary. Some technological trends are important to follow as present and future directions of basic and applied research. The most significant of these are:

- Increasing materials complexity because of increased functionality
- Integration of different materials into multifunctional components
- Miniaturization of devices
- Exploitation of nanosized effects

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- Theoretical treatment and modelling of materials and components development

In addition to these trends, present-day environmental regulations and awareness and the recycling of materials will affect the use of materials and require less expensive production processes.

According to these trends in materials research, a change in paradigm can be observed. Traditional materials-oriented research is now complemented by more interdisciplinary and method-linking work, while at the same time the different hierarchies of length scales are also considered (Fig. 1.7). Size hierarchies extend from the architecture of structures at the atomic and molecular scale (via microstructure characteristics in nano- and microsized dimensions), up to macroscopic features of components and devices. One fundamental area of research to pursue is the development of a unified description of deformation and fracture in order to design microstructures for improved mechanical reliability of ceramic parts. This would decrease the material's susceptibility to environmental stresses and facilitate integration of ceramics into whole engineered systems. In addition, as these tasks become more and more interdisciplinary, advances in ceramic materials will benefit increasingly from closer cooperation among materials scientists, physicists, chemists, engineers, and, especially, biologists.

1.2.4. Needs for Future Basic Research

Following technological trends, the needs for future basic research in the field of ceramics can be divided into four major areas: *(a) materials and materials properties* research in order to widen the area's scope and match its needs for future applications, (b) research to increase the knowledge of economical and ecological *production processes for materials, components, and devices, (c) miniaturization and integration, and (d) modelling and numerical simulation*, which would complement or even act as a substitute for present areas of experimental work, thus not only directing research to defined questions, but also reducing practical work and time periods typically combined with product development. The identified four areas of future basic research will be discussed in the following.

(a) Materials and their properties

Ceramics now cover an extensive area of functionalities. Hardly any other class of materials offers such a variety of properties useful for applications. Promising technical developments emerge from the discovery of new compounds, and new materials with specific functions have recently appeared on the horizon. These materials include high-temperature superconductors, ultra high-strain single crystal piezoelectrics, high-frequency dielectrics, phosphors, intercalation compounds, ductile layer-structured ceramics, and thermoelectrics. Detailed basic research in solid state chemistry and solid state physics (i.e., activities fo-

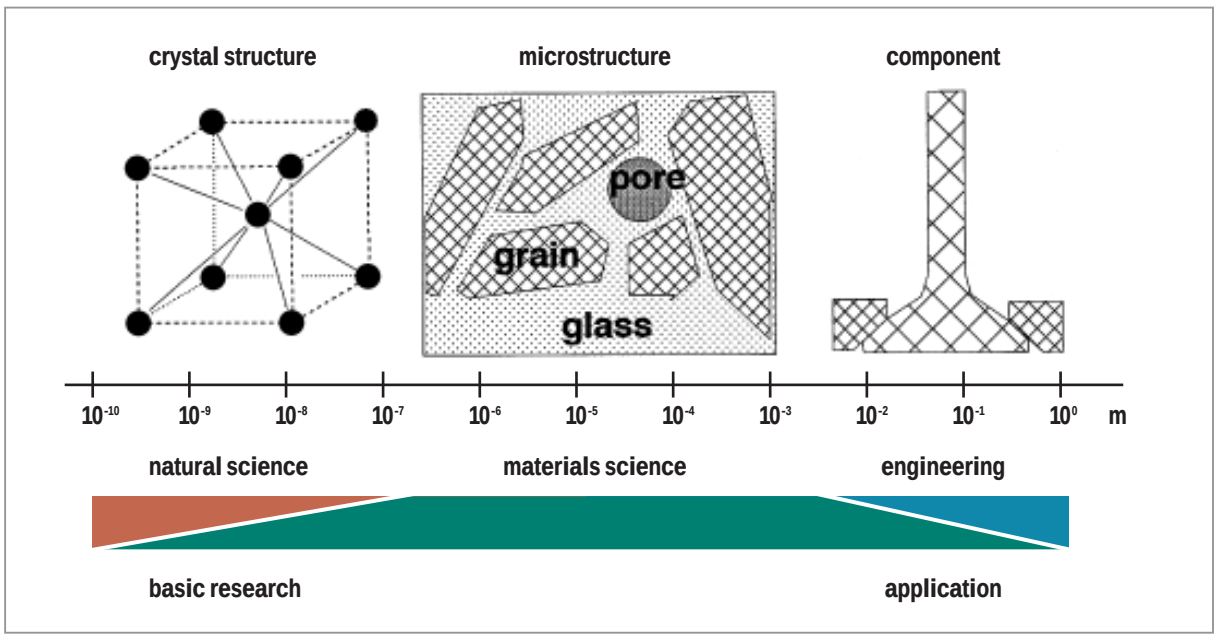

Fig. 1.7. Hierarchies of length scale and multidisciplinary character of materials.

cused on the elaboration of new compounds and the understanding of their basic properties) will continue to widen the scope of materials, resulting in the optimization of existing materials' functionalities and the likely enhancement of ceramics with new physical behaviours. Since both result in complex materials, there will be a continuous need for the comprehensive evaluation of the underlying materials (i.e., structure analysis and phase studies of multicomponent systems). Therefore, extended investigations of physical, chemical, and mechanical properties will be necessary in order to evaluate the potential of the materials for practical applications. Of special interest will be the investigation of nanosized effects onto certain properties (i.e., continuous or discontinuous property changes with size decreases and completely new physical behaviours).

In the area of ceramic materials, ferroelectric ceramics are technically the most important. They are known for their unique properties, such as high dielectric permittivity as well as high piezoelectric constants, and are used in multilayer capacitors or as microwave devices within wireless communication systems. Besides that, they will very likely play a key role in the future of information technology as a basis for low-cost, low-power energy consumption, high-density storage, and fast readout of information. Most of the inorganic materials for linear and nonlinear optics are also ferroelectric. Infrared absorption, pyroelectricity, acousto-optical activity, second-harmonic generation, electro-optical modulation, and photorefractivity are optimized in ferroelectrics because of their strong linear and nonlinear polarizabilities. However, the increasing power and speed of today's lasers has a large effect on the crystalline quality and defect content of ferroelectrics. This is even more crucial in the case of integrated devices for which optical density, electric fields, thermal gradients, and mechanical stresses are increased by the limited size of wave guides.

Presently, piezoelectric ceramics certainly show the broadest range of individual applications, including sonars, ultrasonic cleaners, buzzers, accelerometers, hydrophones, surface acoustic wave filters, delay lines, piezotransformers, ultra-precision positioners, and many other sensor and actuator functions requiring a wide field of interdisciplinary research for further evaluation.

Magnetoresistive materials, which change their electrical resistivity upon application of magnetic fields, have also received attention for magnetic reading heads. Ceramics, such as doped rare-earth manganites (in which so-called phenomena of colossal magnetoresistance were observed) exhibit extremely high values for this effect, even superior to that of giant magnetoresistant metals presently in use.

Ion conduction also provides great technological benefits. It is a basis for energy and information technology systems such as batteries, fuel cells, chemical sensors, and chemical filters providing efficient and cleaner energy transformation, chemical control, and environmental protection. Apart from the functional aspect, the application of these materials requires the simultaneous fulfilment of many properties. These include thermal stability, chemical stability, mechanical stability, and electrical stability. Examples in which fundamentals led to new materials and devices are stable proton conductors, interfacially controlled ionic conductors, and chemical sensors for acid/base active gases.

In the field of high-temperature superconductivity, important progress has been achieved over the last few years regarding both energy applications as well as electronics. Large-sized demonstration prototypes of superconducting cables, transformers, and fault-current limiters have been fabricated and successfully tested. Some products, such as current leads for low-temperature systems and filters for mobile telephone base stations, have already been introduced into the market in a competitive way.

Characterized by a steady increase in energy density imposed by phenomenal requirements in the thermal management of last-generation integrated semiconductor devices, highly thermal conductive materials represent a more important class of functional ceramic materials.

There is much room for development in basic research, not only in functional materials, but also in structural materials. Superhard materials for cutting tools, abrasives, and tribological applications, as well as thermal barrier coatings to improve gas-turbine efficiency, and fibre-reinforced ceramics for failure-tolerant high-temperature components, are just a few examples of great technological importance.

A unique set of properties is exhibited by a newly identified family of ternary-layered hexagonal carbides and nitrides (e.g., Ti_3SiC_2). These ceramic compounds are malleable at room temperature and deform plastically at elevated temperatures. They warrant further research.

Other important classes of ceramics to be studied both for functional as well as structural applications are negative- and low-thermal expansion materials such as beta eucryptite, sodium zirconium phosphates, vanadates, and tungstates. There is a widespread need for these materials in applications that require either dimensional stability or thermal-shock resistance as well as in electronic devices, mechanical parts, catalyst supports for automotive applications, high-performance optical mirror substrates, ceramic

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hosts for nuclear waste immobilization, port liners for diesel engines, and coating materials for C/C composites.

(b) Processing and microstructural design

Ceramics are synthesized into glasses, polycrystals, and single crystals, and many forms dictated by their use, including fine powders, fibres, thin films, thick films, coatings, monoliths, and composites. Polycrystalline components are conventionally produced by powder synthesis and forming processes followed by sintering at high temperature. The performances of ceramic materials are determined not only by the structure and composition, but also by defects (such as pores), second phases (which can be deliberately added to facilitate processing), and interfaces. Thus, one of the primary limitations of current ceramic processing technologies is that they are an art as well a science. This situation is changing progressively. For instance, in order to meet the requirements of miniaturization and integration, these techniques have to be supplemented by deposition techniques, such as physical vapour deposition (PVD), pulsed-laser deposition (PLD), chemical solution deposition (CSD), and chemical vapour deposition (CVD). During these processes, the materials are synthesized on a microscopic scale without powder processing as an intermediate step, usually at temperatures much below the typical sintering temperature of bulk materials. Not only can ceramic materials of small dimensions (e.g., the size of semiconductor chips) then be deposited, thus responding to the integration needs of different materials, but their ceramic compositions and structures can also be designed much more flexibly. The understanding and mastering of phenomena at the microscopic and, more importantly, at the nanoscopic scales clearly need further basic research. A specific example can be found in thin films of ferroelectrics, where dielectric properties are dominated by interfacial effects rather than by the bulk capacitance.

A great challenge is the architecture of ceramic materials in atomic dimensions, not only in thin films but also in thick films and bulk materials. The ceramic materials will open up novel classes of materials with properties still unknown with respect to conventionally processed materials. One possibility for research is the thermally induced transformation of preceramic compounds by solid state thermolysis (SST). By tailoring the composition and molecular structure of precursors by means of advanced chemical syntheses, and by controlling thermolysis, the composition, structure, and microstructure of ceramic materials can be designed. The characteristics of precursor thermolysis, and the relative ease with which various geometries can be processed at the preceramic stage (such geometries include fibres, thin films and coatings, infiltrates, bulk materials, etc.), using standard polymer processing techniques, makes them highly applicable for the production of fibre-reinforced composites, oxidation-resistant coatings, wear-resistant materials, and many others.

Another growing field of research with an attractive technical potential is the production of materials inspired by biomineralization. Oxidic deposits from aqueous solutions on organically modified surfaces, for example, provide a synthesis route for ceramics at ambient conditions. Such template-induced and self-assembled materials using biomimetic techniques provide “soft,” low-cost routes, offering real opportunities to get new metastable materials that possess original microstructures as layered polymer-ceramic composites and cannot be obtained by conventional high-temperature routes. Therefore, the investigation of interactions between organic and inorganic phases, as well as nucleation and growth phenomena, is a promising area of basic research.

Nevertheless, conventional elaboration processes will continue to offer breakthroughs. A deeper understanding of the surface chemistry of powders will lead to a better control of the interaction between particles during colloidal powder processing, thus providing a means for controlling powder consolidation and defect-free microstructure. New methods for net-shape forming based on the control of interparticle forces in dense suspensions of powders have been proposed recently. There is no doubt that possibilities offered by surface chemistry are far from being fully exploited, especially in the case of nonoxide ceramics. Among the challenges for future years is the development of processing paradigms for the production of finer powders, which could lead to new applications resulting from different green-state architectures.

Direct and indirect cost savings by process-cost reductions and product improvements, respectively, are necessary in the field of advanced properties of ceramics. Cost savings are typically achieved by a better understanding of the fundamentals of the underlying processes. Savings could also be obtained by new types of low-cost processes, component design changes or simplifications by using proper joining techniques, or product-development time reductions (e.g., by rapid prototyping). In essence, processing science remains a net priority, but in the case of ceramics, it now extends far beyond the simple processing of powders.

(c) Miniaturization and integration

One of the great challenges and opportunities in advanced processing lies in the miniaturization and integration of different classes of materials (e.g., ceramics, metallic alloys, polymers). Miniaturization requires a search for new

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processing techniques adequate for the manufacturing of miniaturized components and devices, but also a proper means to control microstructure at the mesoscopic level. A new field of research emerges as many characteristics reveal side effects at the mesoscopic dimension. For instance, the properties of thin films and nanostructured materials often deviate from those of corresponding microstructured bulk materials.

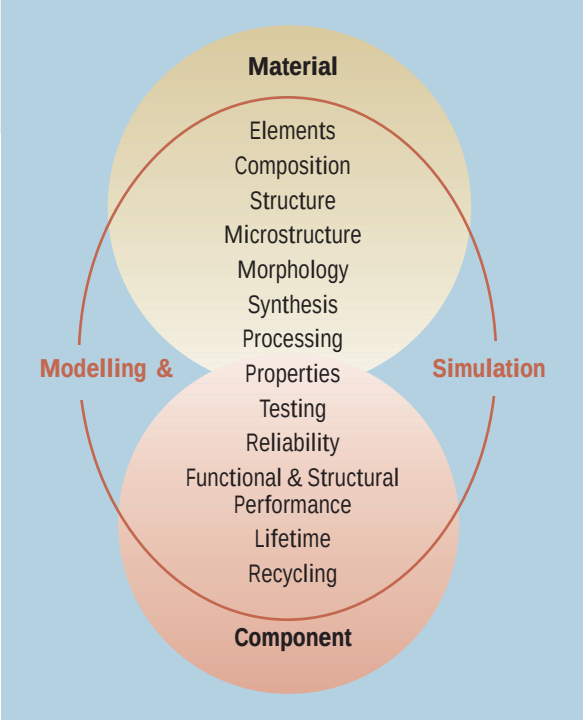

Fig. 1.8. Modelling and simulation in material science and engineering.

Due to miniaturization, nanosized effects and nanotechnologies will thus gain importance. The miniaturized devices may include ultrathin films, multilayers, interface controlled materials, nanocomposites, metastable systems with high information content on the nanoscale, and lateral nanostructuring. Therefore, miniaturization provides an innovative means for system development.

Furthermore, present challenges to technological development often lie in engineering the miniaturized devices. Integration of different ceramic materials with metals or future polymers is one way to miniaturize systems and to produce one "function" for both functional and structural applications. Integration will thus play an increasing role in many technologies. In the case of microelectronics, for example, driving forces are the integration of various functions into conventional semiconductor chips and the evolution of multifunctional components and systems. The area of integration would benefit from a clear understanding of effects that occur during the co-production of different materials in a single device, and also of the role played by interfacial chemistry in adhesion and fracture. Concerning microelectromechanical systems (MEMS) all scientific background of mechanical behaviour must be revisited for two reasons: (1) classical fracture mechanics may not be appropriate at the microscale when the size of the component approaches grain size; and (2) the validation of the design will require new testing methodologies for strength, toughness, fatigue resistance, etc.

(d) Modelling and numerical simulation

Modelling and simulating have been used for a long time in the development and improvement of materials. On one hand, atomic dimensions have been successfully described by, for example, first principle and *ab initio* quantum concepts. Fundamental theories exist for many physical phenomena (e.g. elasticity, plasticity, fracture, thermodynamics, electricity, magnetism), all of which improved enormously the understanding of materials. On the other hand, there have been developed a variety of chemical continuum concepts and macroscopic finite element methods to simulate the behaviour of materials and compounds. Both areas have created much progress in materials science and technology (See chapter 4). However, in order to achieve a real breakthrough in designing new materials and tailoring their properties, there is a need to bridge both areas. The most desirable breakthrough would be to outline the structural and functional performance of a material directly from its elemental composition, structure, and morphology (Fig. 1.8). Modelling concepts, which cover a complete sequence from the state of matter (via material synthesis and processing) to a component's properties and performance, would be the most desirable in materials science and engineering.

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1.3. Advanced Ceramic Materials: Summary of Possible Applications

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1.3.1. Introduction

Ceramics, which exhibit very specific properties and cannot be replaced by other materials, play a significant role in the performance of numerous devices and equipments. In order to tailor a device property to its function, a good knowledge of the correlation between property and microstructure is required. Because the microstructure depends on the processing route, ceramic processing methods are decisive factors in developing the ceramic market.

While current ceramic applications are well known, scientists in the field continue to develop novel processing methods that can produce components of a complex shape and high reliability with a minimum of machining and at a lower cost.

1.3.2. State of the Art

The current status of research and development concerning materials and composites has recently been described [1-4]. In this chapter, we focus on areas of emphasis for new materials, new applications and areas for application, and new processes.

Many new materials are worth further examination, some of which are mentioned below:

- Research activity in *inert or active bioceramics* has been significant and will have an effect in the medical and health fields, prompting new actions for the future. Abrasives for cut-off or grinding wheels and cutting tools for metalworking are important for industrial applications, and not enough research is dedicated to these materials. Therefore, *hard and superhard ceramics* are worth studying more extensively.
- Methods for studying the high-temperature behaviour of *particle filters*, corrosion behaviour in particular, need improvement. Decomposition of SO_X and NO_X, pollutants resulting from the combustion process, must be realized through catalytic reduction at low temperature.
- *Ceramic membranes* are very useful for liquid (water) or gas hyperfiltration at a molecular scale.
- *Electroceramics* have a wide range of applications and correspond to significant research activities in the fields of ion-conducting ceramics (such as *batteries and sensors*), electrical insulators (substrates and multilayer integrated circuit packages), semiconductors (*sensors*), and superconductors.
- *Ferroelectric ceramics* are very promising for many applications such as capacitors, sensors, piezoelectric transducers, electrooptic devices, and thermistors, giving rise to productive research activities.
- *Ferromagnetic ceramics* play a significant role in the electronics industry, and their applications are extensive, including recording, telecommunications, televisions, and electronics.
- *Miniaturization for electroceramic components and devices* must be a priority for the future.

Chemical, physical, and mechanical characterization techniques have been suitably developed for materials applications. Using these tools, we need to explore new areas of materials application, some of which are listed below:

- In *transport*, catalyst supports for purification of automobile exhaust fumes are now finalized, but *particle filters* for diesel engines need further investigation to take into account corrosion problems. The monolithic or fibre-composite *ceramic brakes* for trucks, trains, planes, and automobiles require further development in terms of lifetime, cost, and performance. The use of other components (such as valves, seals, turbocharger rotors, cam rollers, tippers, etc.) is actually limited because of cost and reliability problems. Components for *gas-turbine* power generators have to be improved. Major efforts are being made to develop a high-efficiency *solid oxide fuel* cell.

- For *energy production*, several routes using coal, gas, or nuclear fuels are being considered. The performance of coal plants are limited by the thermomechanical and chemical behaviour of *refractories*, and a better knowledge of this behaviour is needed. Improvement of combustion turbines requires an improvement in the behaviour of used ceramics, the use of more efficient *thermal barrier coatings*, and a decrease in cost. The problem of how to clean up radioactive *waste* from nuclear power plants must be solved. Environment factors to take into consideration include type and quantity of waste, health risks, level of pollution, and route of contamination

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(soil, water, air). Fibres, whiskers, chromium oxide, and small particles can be carcinogenic, and substitutes must be found.

- The *building industry* has a significant influence on people's lives and more emphasis needs to be placed on research. Materials that are important include cements, concretes, gypsum cements, roof tiles, and bricks. Traditional ceramics are used throughout industry, but their development is hindered by the lack of interest in ceramic processing technology and its role in microstructure and properties. An area of growth is ceramic heritage, an application used to preserve and restore buildings, monuments, etc., which is interesting more and more researchers.

Several processing methods are well developed, including the characterization of powders, microstructure, and porosity; others need more attention:

- *Powder synthesis* requires complementary studies, the powder behaviour being fundamental for shape-forming processes and densification. Some shape-forming processes, such as pressing, slip casting, and tape casting, are well known. Sintering has been extensively studied, and there is a good understanding of the involved mechanisms for ceramics. "*Modelling*" *density variation* during pressing and shrinkage during sintering are needed in order to obtain near-net shape parts and to minimize machining, which represents a large portion of the fabrication cost.

- *New routes for near-net shape* forming of advanced ceramics and composites have been developed and hold promise for the fabrication of components with high reliability at acceptable costs.

- Injection moulding offers great promise for low-cost fabrication but needs more attention in the area of *organic vehicle removal*.

- Pyrolysis of inorganic polymers can be used for the production of ceramic parts, but this process results in significant shrinkage, which can lead to the introduction of flaws. Therefore, this route is promising but requires further research concerning the synthesis of *inorganic polymers* and the transformation of polymers to inorganic solids.

- Quality control methods for ceramic components are not often studied. The area of *nondestructive techniques*, in particular, needs more attention.

Compared to those of the U.S. and Japan, the EU's fundamental research activities have been quite effective in the areas of processing, bioceramics, ceramic matrix composites, carbon-carbon composites, cutting tools, nuclear ceramics, and electroceramics, but rather low regarding filters, building materials, refractories, fibres, gas turbines, abrasives, superhard ceramics, nanomaterials, function gradient materials, and finishing.

The EU, U.S., and Japan have different research strategies. In Japan, national projects with technological goals are defined and funded by the government. A similar approach for some programmes exists in the U.S. In contrast, European projects are rather broad with less precise goals, but there are national projects with more specific objectives.

1.3.3. Trends for the Future

The socioeconomic impact of the following themes will be taken into account in establishing priority actions and basic research necessary to reach fixed objectives which are summarized in Table 1.1 and 1.2.

(a) New materials, devices, and applications

The following are considered priority actions:

i) Bioceramics: application to health Today's orthopaedic implants have an *average life expectancy of 10 to 15 years*, which is generally limited by osteolysis, which is caused by the wear of polyethylene cups against metal or ceramic (i.e., alumina- or yttria-stabilized zirconia) femoral heads. However, considering our aging population, there is a growing demand for implants with *a life expectancy of more than 30 years*. They must include new generations of ceramic-ceramic wear couples for hips, and knee prostheses that can last where ceramics have so far failed.

Therefore, existing ceramics must be improved in terms of *reliability* (resistance to slow crack propagation for alumina-based materials and stability, and in particular for zirconia ceramics, which presents a problem for surface low-temperature degradation). When working on *ceramic processing*, scientists must strive to refine microstructure (colloidal and sol-gel) processes and increase ceramic stability and crack resistance. Ceramic processing must include the ability to *make complex shapes* (i.e., knee prostheses) with high reliability. We must incorporate new ceramic materials into orthopaedic design. They must address current biocompatibility problems and have properties superior to monolithic alumina and zirconia. There is a new interest in the potential for the biomedical applica-

tions of zirconia-toughened alumina. Materials scientists are already familiar with *zirconia-toughened alumina*, which is exceptionally hard, strong, and crack resistant. However, its superiority for joint prosthesis application must now be proved by simulator studies under physiological conditions (where there is a need for knee prostheses simulators and complex modes of fracture studies), industrial manufacturing, and *in vivo* preclinic evaluation.

Bioactive ceramics, mainly hydroxyapatites, are used today as coating on femoral stems and acetabular cups for noncemented hip and knee joint prostheses. However, their use must spread to other applications, such as bone substitutes. Most orthopaedic surgeons agree that synthetic bone substitutes sometimes result in clinical failure caused either by materials fracture or lack of bone integration. The challenge is therefore *to tailor the microstructure and the composition* (hydroxyapatite/tri-calcium phosphate composites) of bone substitutes to adapt to the biofunctionality in a given site. Materials scientists should also work with biologists and surgeons to better understand osteoconduction mechanisms to back-up processing. The second generation of bone substitutes must be more active, incorporating *medicines* (e.g., antibiotics, chemotherapy, drugs) to act locally against disease. The third generation will be the *hybrid bone*, where the ceramic is the support to human cell culture. *Basic research in bioceramics* should focus on producing complex shapes with high reliability, developing nanocomposite ceramics with improved properties, and incorporating medicines into hybrid bone.

ii) Ceramics and environment The reduction of pollutants, an actual necessity, requires research work in the following areas:

- *Particle filters:* The corrosion behaviour must be improved by acting on the ceramics microstructures, decreasing the glassy phase amount, or changing the type of ceramic (oxide or nonoxide ceramic). Furthermore, filter materials must show good thermomechanical behaviour.
- Development of a *low-temperature catalytic reduction* for the decomposition of SO_x and NO_x pollutants.
- Problems of *refractories* used in *waste* treatment plants and treatment of flying *ashes*.
- Development of new ceramic *membranes* for hyperfiltration and nanofiltration of liquid or gas, often very aggressive, for desalination.
- *Nuclear waste* treatment: vitrification, and cementitious materials.
- Ceramic *recycling*.
- Development of *antibacterial* tiles, new sanitary wares, or smart toilets.

Priority research in environment must be focused on catalytic reduction, filters, membranes, nuclear wastes, recycling, and antibacterial actions.

iii) Nanomaterials and functional gradient materials It is expected that nanostructured ceramics play an important role in following areas:

- *Nanocomposites* are known to exhibit unusual properties. Creep resistance, and thermomechanical or wear behaviour can be improved by using nanocomposites. Nanocomposites or nanoceramics exhibit superplasticity, which can be used for shaping.
- *Nanostructured coatings* on substrates allow increased wear and corrosion resistance and durability of *cutting tools*. The different processes used for obtaining nanostructured materials and nanomaterial behaviour must be investigated further.
- *Carbon nanotubes* show exceptional mechanical and electronic properties, and can be very high-performance materials. This new class of materials merits greater attention.
- *Functional gradient materials* reduce thermal stresses for thermal barriers and can be used in a number of applications, including thermal insulation, thermal fatigue, oxidation and corrosion resistance, and electrical, magnetic, or optical properties. Research activity in *functional gradient materials (processing and properties)* must be encouraged.
- *Superhard* ceramics are interesting materials, but research in this range is insufficient.
- *Ceramic-ceramic* and *ceramic-metal joining* is important for the production of complex structures and requires further development.

Preferably, *research in nanomaterials* should focus on nanostructured coatings and carbon nanotubes.

iv) Electroceramics *Electroceramics* are subject of broad interest to the research community. The following are some of the areas of electroceramics that merit increased attention: *piezoelectric actuators*; hybrid s*ensors; electrooptic* devices; new *ferrites*; resistors; positive temperature coefficient materials; materials for batteries, fuel cells, and electrochemical capacitors; oxygen separation membranes; transport properties; and defect chemistry.

Research in the following areas must be developed:

- *Nanopowders, nanoelectroceramics*
- Decrease of the sintering temperature
- *Multilayer structures*: reduction of thickness, substitution of noble metals
- Decrease of the mechanical and dielectric loss at very high frequencies

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R & D tasks		Socio-economic impact
• Microstructure and composition tailoring • Corrosion • Science of interfaces • Miniaturization • Modelling	**New materials** Bioceramics Filters and membranes Nanomaterials Electroceramics	• Health • Environment • **Structural and functional ceramics** • Wireless technologies
• Low cost • Removal of organic vehicle • High reliability • Modelling	**New processes** Near net shape forming Injection moulding Green machining Self-propagating high temperature synthesis	• Complex shape parts • Structural and functional ceramics
• Life-time (fatigue, oxidation) • Reinforcement • Recycling • Repairing • Modelling	**New applications** Thermostructural composite parts Brakes Refractories Nuclear wastes Building and traditional ceramics	• Aerospace • Environment • Energy • Transport • Metallurgy • Everyday life • Heritage

Table 1.1. The socio-economic impact of ceramic materials.

- Development of sol-gel technology for thin layers
- New ceramics with improved properties
- New processing routes
- *Miniaturization* of components and devices for wireless technologies

In the area of *electroceramics*, particular attention must be devoted to sensors, actuators, electro-optic devices, superionic conductors, ferrites, nanoelectroceramics, multilayer structures, and miniaturization in relation to new processing routes.

The *science of interfaces* is multidisciplinary and useful for a wide spectrum of applications, such as electroceramics, functional gradient materials, joining, thin films, and coatings, and therefore needs more research, particularly in the areas of miniaturization and nanomaterials.

(b) New processes

A significant challenge in ceramics concerns the fabrication of *complex-shaped components* without defects (pores, inclusions, inhomogeneities, etc., which increase the risk of failure), with *high reliability* and *low cost*. Because machining is expensive, it will be important to develop and optimize *near-net* shape forming of ceramics, which allows minimizing of fabrication time, a primary competitive factor. Processing routes requiring more research include:

- *Injection molding:* This process needs a large amount of binders that must be removed without leaving flaws.
- *Colloidal techniques:* Direct coagulation casting, gel casting, and hydrolysis- assisted solidification, which need a high amount of additives.
- *Solid freeform* fabrication.
- *Temperature-induced forming:* Consolidation of a slurry is obtained by a temperature increase, and shaping is made by using a nonporous mold.
- Directed *molten metal oxidation* or reactive melt penetration for composites processing.
- *Self-propagating high-temperature synthesis* is an interesting, low-cost technique for making fine powders.
- Synthesis and processing of *nanomaterials and nanocomposites* are exciting areas to be developed.

The *machining* of sintered ceramics is time and energy consuming and can represent up to 80% of the production cost of a ceramic part. A possible route to reduce machining costs is to machine green ceramics, which can be an effective way to obtain complex ceramic parts. However, research in this field is sparse and needs to be developed. It is critical that the research community investigates the types of *green properties* required to withstand green machining. The *role of binders* must be specified, and specific mechanical tests for green compact characterization must be developed in order to find the correlation between mechanical behaviour and green machine performance.

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Basic research in processing must be devoted to near-net shape forming, organic removal, SHS synthesis, and nanomaterials.

(c) Other applications

i) Fibre-reinforced ceramic composites Ceramic matrix composites reinforced with fibres (CMCs) are devoted to *high-performance thermomechanical applications* without the brittle fracture behaviour typical of conventional ceramics. For the future, the main obstacle concerning these materials is still costs of both, raw materials and manufacturing. In addition, several properties (such as *oxidation resistance, creep, and fatigue*) have to be improved. Research must be developed in the following directions:

- *Reinforcement:* There is a need for cheaper fibres with improved creep resistance. The best SiC fibres are very expensive and exhibit extremely high creep and oxidation rates. Oxide fibres, like alumina, are limited because of very high creep rates. Carbon fibres need improved oxidation-protection solutions.

- *Protection against oxidation:* Development is needed of sophisticated multilayer matrices and multilayer *surface coatings* in order to promote the *matrix cracks healing* by formation of glasses in the whole temperature range. Research in this field must be done in close relation with processing solutions. Brake materials (carbon-carbon or other systems) need research in a similar direction, with particular attention to the effect of the inhibitors on friction performance.

- *Reliability of inhomogeneous, anisotropic, and porous materials:* Development is needed of adapted nondestructive examination methods, *specific strength and quality criteria*, and new *damage indicators*. Despite the effective reduction in brittleness caused by fibrous reinforcement, further research is needed to improve toughness and thermal and mechanical *shock resistance*. This is particularly true in light of the goal of cheaper materials.

ii) Refractories Refractories are largely used in industry-iron, steel, metallurgy, foundry, cement works, glass, ceramic, power plants, chemistry, etc. These materials play an important economic and strategic role, and the improvement of their performance constitutes a major challenge for the future. Traditionally, rather empirical methods were used to improve refractories' behaviour, but it is now very desirable to *forecast* and *model microstructures and properties of refractories*.

We must encourage the study of the *microstructure-property* relationship, *modelling* of the thermomechanical response, and *corrosion* behaviour and apply our results to real components.

Needs in basic research for ceramic materials

• Near net shape forming	• Nanomaterials and nanocomposites
• Processing of complex shapes with high reliability	• Nanostructured coatings
• Hybrid bones	• Sensors
• Catalytic reduction	• Electro-optical devices
• Membranes	• Superionic conductors
• Nuclear wastes	• Ferroelectrics
• Recycling	• Miniaturization
• Antibacterial actions	• Multilayer materials
• Nanopowders	• Interfaces
• Carbon nanotubes	• Self healing composites

Table 1.2.

iii) Building materials Because the use of cement requires water consumption, the availability of water is critical. It is therefore necessary to improve the *workability of concrete* in order to reduce *water consumption*. Macrodefect-free cements with *organic additives* have more strength and lower porosity than conventional concrete. Cement strength can be increased by fibre reinforcement. Recycling fly ashes and other *light aggregates* in concrete must be encouraged. The ability to use cement for *repair or reconstruction* now needs to be taken into account. The *temperature behaviour* of cement and concrete also needs to be studied and improved for public safety in tunnels, buildings, and other public structures.
Research on cement, concrete, and plaster must receive increased attention. Specifically, the following areas need *basic research*: self-healing composites, fibres, interfaces, corrosion, recycling, and new concretes.

In conclusion, new developments in ceramics require both basic and applied research in materials and properties, processing and microstructure, and design and modelling of materials and devices. The trends for the future are summarized in Table 1.2.

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1.4. Inorganic Materials

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1.4.1. Introduction

All solids, whether natural or synthetic, are materials. However, when we speak of the science of materials, we are speaking of the relationship between structure and properties such that structures can be selected and constructed to have the desired properties. This definition encompasses inorganic as well as molecular materials.

The preparation and examination of new solids have led to technological advances as well as enormous progress in our understanding of materials properties. We now know that the behaviour of ions, atoms, and molecules within various types of solids can be (and usually is) drastically different from the behaviour of the same species as individuals. This is somewhat analogous to the behaviour of humans as members of various groups (ranging from an informal company at a party to a well-organized sports team or military detachment) and as solitary "individuals."

Over the last thirty years, chemistry has made an increasingly important contribution to the science of materials, so much so that the terms "solid state chemistry" and "materials chemistry" (which includes inorganic and molecular materials) have come into being.

The guiding principle for all fields of study in materials science is that the selected function defines the material, and each of these fields of study requires a multidisciplinary approach, ranging from fundamental research to creation of the final product (Fig. 1.9). The main goal of this chapter is to show the state of the art, visions, breakthroughs, and research needs in three basic complementary materials science research fields:

- Inorganic solid state chemistry and materials chemistry
- Inorganic molecular chemistry
- Inorganic amorphous solids (glasses)

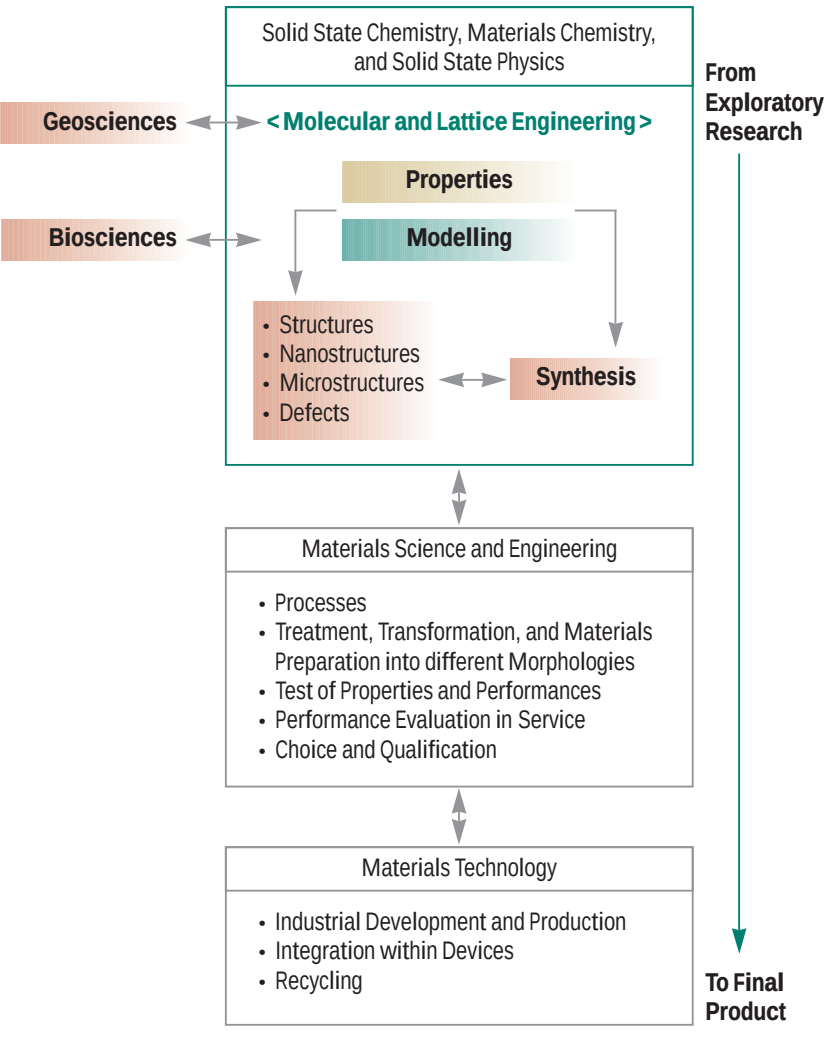

Fig. 1.9. Selected functions define the material.

1.4.2. Inorganic Solid State Chemistry and Materials Chemistry

Inorganic Solid State Chemistry provides the background needed for fundamental chemical research to improve existing materials and provides the basis for the discovery of new materials through the use of chemical and physical-chemical concepts (e.g., structure, chemical bonding, etc.) at the atomic scale. Lattice engineering chemistry could be synonymous with solid state chemistry. On the other hand, materials chemistry is a research field concerned

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with understanding and controlling functional condensed matter from a chemical perspective. Solid state chemistry, materials chemistry, condensed matter physics, and engineering constitute the main components of the multidisciplinary materials science research field.

(a) State of the art

Solid state chemistry has two well-defined faces: *a static face*, which is the determination and description of the properties of a given material in terms of geometrical structure, electronic structure, chemical bonding, and physical properties; and *a dynamic face*, which describes any kind of time-dependent structural, compositional, or electronic reorganization in materials, in particular reactivity, as a functional property of chemical systems. In the area of solid state and materials chemistry, considerable progress has been achieved in the understanding of the correlations between structure, bonding, and physical properties. However, understanding the most important relationship – the one between these static parameters and the dynamic aspects (the reactivity of solids) – is far less developed.

Chemical bonding in solids is not completely understood, mainly because of the wide variation in elemental chemical properties. Many difficult challenges remain in predicting the composition, structure, and properties of new materials. Consequently, the synthesis of novel solids is as much an art as a science. (It should be noted that the discoveries of new compounds and structure types highlight a versatility that nature has allowed with a relatively small number of elements.)

Research in the field of inorganic materials chemistry during the last decade has been mostly directed towards very relevant developments in some groups of materials. Important discoveries concern high-T_c superconductors, the fullerenes C_{60} and C_{70} (and related carbon or inorganic fullerides), colossal magnetoresistant manganese oxides, and mesoporous solids with catalytical or adsorbent applications. In addition to these discoveries, which have led to a vast number of articles published in the most prominent journals of the field, the following should also be highlighted: fast ion conductors and battery materials, hybrid materials, biomaterials, and dielectric and optical materials. Fundamental inorganic materials chemistry research must be concerned with the following three goals: (1) the development of synthetic methods to prepare novel compounds or to improve their properties, (2) the discovery of new phases with desired properties from crystal chemical criteria, and (3) the full characterization of new phases from a chemical and structural point of view.

Over the last thirty years, Europe has had an impressive record in the sciences, winning Nobel Prizes in both chemistry and physics. During this time, European solid state chemistry and physics have acquired an international reputation because of consequential contributions in the domains of, most particularly, magnetism, superconductivity, theory of metals and semiconductors, organic conductors and superconductors.

For the past twenty years, the fields of solid state chemistry and physics have grown together. Researchers from both disciplines have tried to establish a common language that not only defines a material in terms of its structure, composition, defects, and morphology, but its physical properties as well. Competition among countries has in fact brought collaboration between the two disciplines, specifically collaboration between the earlier discipline of materials for optics, optoelectronics, and electronics, and the more recent discipline of superconductors with a high critical temperature. In a similar way, the recent emergence of the nanosciences (influenced by trends in chemistry as well as physics) has brought to light the complementary relationship that exists between physics and chemistry.

Europe still holds the international standard in solid state chemistry and physics, mainly because of its strong emphasis on both education and research. The United States, influenced by educational institutions in France and Germany, has not yet achieved its potential for leadership in solid state chemistry, particularly in the realm of education. Japan, known for its mastery of materials technology and the transformation of fundamental discoveries into products, compensates for lost time in basic research through its achievements in solid state chemistry and molecular sciences.

A fundamental difference between Europe and the U.S. and Japan exists in the influence of industrial groups (such as Dupont de Nemours in the U.S. and Hitachi in Japan) on the global effort in basic research in materials. It should also be noted that in the past few years, this corporate influence has strongly been reduced but nonetheless remains significant. The U.S. and Japan have recently launched very important nanotechnologies research programmes, which includes nanomaterials. China and Korea have kept pace with Europe, the U.S., and Japan in the fields of solid state and materials chemistry. (It should be noted that the French School of Solid State Chemistry and Physics has formed an alliance with a group of researchers from Asia.)

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The countries of the Central European Initiative (CEI), including Russia, are more oriented towards materials science (e.g., processing, shaping, etc.), but have not yet reached the level of Europe, Japan, the U.S., China, and Korea in solid state chemistry. However, Russian researchers do play a primary role in solid state physics. Unfortunately, despite progress in these scientific areas, the political and economical problems that the countries of the CEI are facing today will certainly impede their development in the disciplines of materials science and solid-state chemistry.

In Europe, France, Germany, and United Kingdom are at the same level of materials science development. In fact, two large industrial groups are strongly involved in these countries' materials science research effort. Spain and Portugal, however, lack behind France, Germany, and United Kingdom. Denmark is a notable contributor to solid state organic chemistry. Italy is active in the field of solid state physics, particularly regarding spectroscopic studies.

Europe has a problem with the valorization of its own research within the European Community. Too many foreign products and technologies are resulting from basic research undertaken in Europe, in France particularly, and then these products are in turn sold in Europe. Japan for instance, is buying the knowledge from Europe at a decreasing rate due to the progress of its own fundamental research. However, it continues to sell the products it has produced with this knowledge in Europe. Europe, on the other hand, buys both knowledge and products. This will ultimately adversely affect the development of research in Europe. We need to decrease both the amount of foreign knowledge we buy and products we sell. Research in Europe could continue to develop if downstream research sectors could find tangible ways to meet the needs of the public. It will be necessary to distinguish between a valorization of knowledge and a solution to scientific and technological problems confronted by industry in the development of a product, process, or technology.

To solve this problem, researchers must convince the public that it is possible to design a product or a process that is cost effective without compromising its state-of-the-art properties (e.g., ability to be recycled, nonpolluting), although cost is not always associated with status. In addition, academic laboratories must help researchers by making available database banks of basic knowledge in order to solve the problems raised by the industry.

(b) Future visions and expected breakthroughs

One of the great challenges in solid state chemistry today is the design and synthesis of novel inorganic solids possessing desired structures and properties. A main focus area is the creation of a suite of tools to predict the stability and properties of a given inorganic network from first principles. Unlike the highly developed field of organic synthesis, solid state chemistry lacks such tools.

To pursue this objective, researchers first need to investigate reaction mechanisms in solid state chemistry synthesis in order to determine the principles that will be the basis for the discovery of unknown materials. It would be advisable to increase the strong collaboration between theoretical activities and experimental efforts for predicting the chemical stability of novel phases and adjusting crystal chemical variables in order to get a desirable physical property. Future research should also study methods for improving existing and new materials to gain a better understanding of the mechanisms responsible for physical properties.

i) In optics The future of materials is found in five main domains: phosphors, scintillators, lasers, and materials for nonlinear optics and colour pigments. The discovery of new materials remains tightly connected with, for example:

- A better knowledge of the nature of absorbing centres, the states associated with charge transfers for phosphors and scintillators.
- The replacement of mercury-vapour luminescent tubes by tubes containing Xe (boosting research on phosphors and identifying levels above 40,000 cm^{-1}, etc.).
- The mastery of vibrational properties (reducing nonradiative transitions).
- The search for nonsolarizable monocrystalline dense materials with unalterable large dimensions, a high quantum yield, and a short lifetime (i.e., within a range of a few nanoseconds) of the level responsible for emissions, mainly for scintillators.
- The search for doped crystals with wide absorption bands for the purpose of compensating the temperature drift of laser diodes.
- The search for "blue" starting from laser diodes emitting red for their application in optical reading.
- The study of nonlinear properties (passive or active planar or cylindrical wave guides [with lasers]), including the origin of dielectric susceptibilities $\chi(2)$ and $\chi(3)$ in glasses and the origin of $\chi(2)$ in certain noncentrosymmetric crystals. Questions to consider include: Are glasses really lost materials for noncentrosymmetric effects? Can they be anisotropic at nano- or microscales? Search for glasses with elevated values of $\chi(3)$ for ultrafast commutation, etc.
- Preparation of dense transparent ceramics for laser sources (IR, etc.).

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- The search for new colour pigments (red to yellow) and anti-UV pigments.
- The optical behaviour of nanometre-sized particles is not well understood, even in common applications involving luminescent, photochromic, and colloid-coloured properties.

Besides the necessity of a better understanding of defects present in single crystals and thin films and of the vitreous state of matter, materials science would benefit from a deeper understanding of the ways in which the study of glass-crystal composition (e.g., the development of vitroceramics) can enhance the development of composite materials for optics (nanograins –> optical nanocavities), the research for new materials, as well as composition and morphology. Hybrid materials, such as organic/inorganic, deserve to be developed (by combining high polarizabilities of molecular entities with good thermomechanical properties of inorganic matrices).

ii) In magnetism Several areas of magnetic materials research need to be explored. Research of new materials is required for permanent magnets, magneto-optical displays, reading heads, etc. A better understanding of the magnetic properties of surfaces and interfaces in *multilayer materials* is also necessary. In addition, the mechanism responsible for giant magnetoresistance in oxides and derived insulating materials is needs to be elucidated.

On a very fundamental basis, it is necessary that the studies of strongly correlated electron systems continue and new, well-characterized materials be prepared (e.g., the effect of the hybridization of 4f or 5f states with conduction electrons on magnetic properties, superconductivity and the heavy Fermion systems, the Kondo "networks" that are still poorly understood, etc.). Furthermore, the possibility of preparing metals and alloys at the nanoscale should allow to address several unanswered questions, such as, what magnetic properties should one expect from a nanocrystalline material for which the fraction of surface atoms is very high?

iii) New materials for passive components (ferroelectrics, piezoelectrics, pyroelectrics, relaxors, etc.) This area of research concerns the preparation of new complex materials (mainly oxides, fluorides, oxyfluorides, nitrides, or oxynitrides) in either stable or metastable form. In the case of metastable forms, the compounds can be stabilized as thin layers thanks to the principle of the method itself, which allows for a pronounced reactivity on the substrate at temperatures that are relatively low when compared to massive materials.

In addition to studies of thin layers and multilayer systems, the effort should also be aimed for bulk materials. As it is for all structural and functional materials, the study of the relationships between composition, nanostructure, microstructure, and properties is mandatory for the understanding of the mechanisms, hence the need for optimizing materials.

These fields of research are very tightly linked to applications: actuators (electrostriction, piezoelectricity), IR detectors (pyroelectricity), and dielectrics for capacitors (e.g., replacement of Pb by other elements). The following application areas require special attention:

- Single crystals and wave guide for optics
- Bulk ceramics, thick films, and single crystals for electromechanical applications
- Electroceramics using ferroelectrics
- Thin ferroelectric films for microwave electronics
- Integration of ferroelectric thin films on silicon for field effect transistor (FET) or ferroelectric memories (FERAM)

iv) Coupling of properties (smart materials) The association of properties (e.g., piezoelectric, piezoresistive, metallic, superconducting, insulating, nonlinear conducting, magnetic, etc.) can be put to good use in granular and nanostructured materials. The modelling of the association of two properties has been achieved without the actual existence of relevant materials. For *ternary nanocomposites*, no modelling exists at all and the materials are scarce.

Similarly, studies on nanocomposites based on fullerenes and carbon nanotubes containing metals or superconductors (e.g., electrochemical deposit in nanopores created by the ionic bombardment of a membrane of soluble polymer) should be developed.

v) Superconductors In the framework of the present programme, research should focus on new compounds rather than those derived from oxygenated perovskites. This recommendation is clearly illustrated by the recent discovery of the high-temperature ($T_c \sim 40$ K) superconductivity of "metallic boron" in MgB_2 (J. Akimitsu, Symposium on Transition Metal Oxides, Sendai, January 10, 2001).

vi) Conductors Three main classes of electronic conductors should be considered (other than metals and their alloys):

- *Molecular crystals* (new charge transfer salts, organic crystals, certain oligometric systems, organic-inorganic compounds, crystals derived from fullerenes). Synthe-

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sis of new molecules must be encouraged, as well as modelling of the electronic properties of such systems.

- *Nanostructures* (molecular wire, carbon, or boron nitride nanotubes, etc.). This is relevant to a totally new domain, and the accent will be put on the research of model systems, on the comprehension and modelling of electronic transport at the nanoscale (which is intrinsically monodimensional), and on the development of techniques that allow such measurements to occur (by means of near-field techniques, particularly STM and AFM).

- *The oxygenated conductors* for which the polaronic nature of the carriers is generally agreed upon but which continue to raise many questions, such as those relative to the role played by magnetic interactions in transport properties (e.g., the effect of giant magnetoresistance on transport properties) or the behaviour in the normal state of superconducting oxides, one of the keys toward understanding the phenomena. New compounds should be prepared and elaborated into single crystals or thin films (oxides, oxynitrides, etc.) in order to study physical properties.

vii) Semiconductors In the next ten years, wide-gap semiconductors will be developed: the III-V nitrides, GaN, AlN for applications in optoelectronics (blue-violet laser), the wide-gap II-VIs (and to a lesser extent ZnSe), and "very large gap" materials and materials with exceptional thermal properties such as BN, diamond C, and SiC. Ternary and quaternary compounds are likely to possess interesting properties, such as the effects of the variation of the magnitude of the forbidden band, which in a given system can go through a minimum as a function of the composition, the so-called "bowing" effect (e.g., GaN-GaAs).

viii) Electrochemical energy storage and electrical energy production Today, electrochemical energy storage and energy production concern batteries and fuel cells, respectively, for many applications (e.g, space, aeronautic and earth transportations, habitats, telecommunications, etc.). Inorganic solid state chemists, electrochemists, and materials scientists are deeply involved in the search for new inorganic materials for applications such as positive and negative electrodes or solid electrolytes in electrochemical devices.

In the field of batteries, two areas can be distinguished by their applications: (1) microbatteries involving inorganic solids (glasses and crystallized materials) for use in smart cards, flat self-powered displays, the healthcare sector, etc.; and (2) batteries for portable devices and electric or hybrid vehicles, etc. In the latter case, interfacial problems can be solved by using a liquid – a gelified or polymeric electrolyte. The challenges are in the effort to improve electrodes presently used and to search for new materials exhibiting high specific energy, rapid kinetic exchange of the ionic species, and a long life (where composition, structure, and morphology of the materials are directly involved). In addition, understanding of electrochemical reactions is also important because chemical reactions occur at all stages of battery use (cycling: calendar life; ageing: shelf life) and lead to materials modifications that must be carefully identified in order to optimize the materials.

In the field of solid oxide fuel cells (SOFC), a great deal of optimism and enthusiasm in Europe that presently exists has resulted from the development of fuel cell technology in the 1960s. The large NASA projects on fuel cells for the Gemini and Apollo space capsules stimulated other fuel cell programmes, in the U.S., Japan, and elsewhere. SOFCs offer a clean, pollution-free technology to electrochemically generate electricity at high efficiencies. These fuel cells roughly consist of an oxygen-ion conducting electrolyte, electronic or mixed electronic/ionic conducting electrodes, and an electronic conducting interconnection.

In addition to technological problems, there are other issues to examine from a materials point of view. The main objective with SOFCs is to operate at the lowest possible temperature (500-700°C) without compromising cell resistance and electrolyte kinetics. The selected materials must fulfill the following conditions: (1) suitable electrical conducting properties required for different cell components to perform their intended cell functions; (2) adequate chemical stability at high temperatures during cell operation as well as during cell fabrication; (3) and minimal reactivity and interdiffusion among different cell components. As of today, yttria-stabilized zirconia (YSZ) and lanthanum manganite or ferrite are the materials most widely used as electrolytes and cathodes, respectively. The challenge is to search for (1) new electrolytes working at low temperatures, and in this manner CeO_2-based compounds should be promising; (2) and new cathodic materials.

ix) Low (reduced) dimensionality materials Nanometric and mesoscopic materials (such as fullerenes, nanotubes, aggregates, nanoporous structures [e.g., silicon and clathrates, composite polymers, etc.]) that continually surprise us by their properties (optical, electric, magnetic, etc.). They must be the topic of study for emerging (e.g., carbon, silicon, boron nitride, etc.) as well as future systems.

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Likewise, new slab-like compounds should be investigated for their superconducting, magnetic, ionic conduction (cationic and anionic) and/or electronic properties. We should focus on their characterization, particularly the occurrence of incommensurate structures.

x) Materials and life sciences The scientific age into which we are moving is a revolutionary one. Biologists will be able to create new forms of life that do not exist in nature (allowing them to identify genetic defects and eventually correct them), and solid state chemists and materials scientists will be able to create a vast range of new synthetic materials that are tailored to meet specific needs. Biologists, solid state chemists, and materials scientists will be able to collaborate in two main domains: biomaterials and materials in relation to healthcare, therapeutics and diagnostics.

Biomaterials – Bioceramics such as polycrystalline alumina, hydroxyapatite, partially stabilized zirconia, bioactive glass, glass ceramics, and polyethylene-hydroxyapatite composites have been successfully used for the repair, reconstruction, and replacement of diseased or damaged body parts, including bones. However, clinical success requires the simultaneous achievement of a stable interface with connective tissue and a match of mechanical behaviour with the implant to be replaced. Research is continuing to develop new coatings that can be chemically bonded directly to the implant material and therefore induce appropriate protein-absorption behaviour so that bone cell adhesion will occur and promote bone formation at the junction site. In a similar way, resorbable biomaterials must be designed to degrade gradually over time in order to be replaced by natural host tissue. To achieve these goals, we must come to a better understanding of the interactions of bioceramics with organic components on the molecular level.

Materials in relation to healthcare, therapeutics, and diagnostics – Living systems are governed by molecular behaviour at nanometre scales where the disciplines of chemistry, physics, biology, and computer simulation all converge. Inorganic nanomaterials can be used in different areas as, for example:

- Substrates for vectorizing (1) contrast-agent molecules in order to improve medical imaging technology, and (2) drugs directly to their site of action by molecular recognition.
- Substrates for biosensors in order to monitor blood chemistry, local electric signals, or pressures. The sensors would communicate with devices outside the body to report results, such as early signals that a tumour, heart damage, or infection is developing. For instance, segments of DNA and other biomolecules can be attached to the surfaces of silicon chips in predefined arrays. This is the basis of so-called "lab on a chip" technology.

One of the main challenges will be to enhance the function of inorganic magnetic nanoparticles or silica chips in order to graft specific biomolecules.

(c) Research needs

Research efforts need to favour *synthesis innovation and materials elaboration within an integrated approach*. The objective of a synthesis can be purely chemical (search for new reactions, new phases) or devoted to materials exhibiting particular properties that could be chemical (reactivity), physical, or biological. However, the synthesis work cannot be dissociated from the understanding of the relationships between structures and properties. Therefore, a particular effort should be made to find new methods of synthesis in order to better master the mesoscopic and nanoscopic aspects of matter. At the same time, we should not overlook any present method that might lead to new stable or metastable materials.

Besides improvement of the synthesis processes and preparation of traditional materials into different morphologies or shapes (such as multilayers, thin layers, crystals, bulky glasses, etc.), it is important *to stress the preparation of materials at the nanoscale*. Thus, we consider on the one hand systems involving one or several components whose dimensions are nanometre themselves, the properties of the obtained systems being exploited at the micro-, milli- or centimetre scale. On the other hand, we will also consider the nanometre systems whose properties are exploited at the nanometre scale and for whom the notion of materials exists at a level as yet undefined.

Another domain where a great deal of expansion is occurring is *hybrid organic-inorganic materials* and *molecular materials*. Important areas of study include:

- The elaboration of materials with new architectures
- The anisotropic growth of phases at the nanoscale as well as at the micrometre scale
- Creation and management of the organization of hybrid systems, most of which are amorphous (e.g., multilayers, slab-like stacking, liquid crystals)
- Preparation of networks with controlled texture and porosity (micro- and mesoporous for membranes, new catalysts, cavities with molecular print)

A better understanding of the forming mode of these systems should allow researchers to achieve enormous

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progress in the field of *biomimetics and materials*. One objective for this field is to understand and copy the modes of mineral growth within cells and living beings in order to develop new materials and systems. This field of research is still very young and suffers from several drawbacks, for which we cannot compensate without a strong collaboration between solid-state chemists, biologists, and physicists. These apparently separate disciplines can complement each other in projects concerning hybrid materials with modulable mechanical properties, adaptive hybrid materials (e.g., photoactivity), hybrid materials for nonlinear optical properties and "photochemical hole burning" (PHB), electrochromic hybrid materials, ionic conducting hybrid copolymers, etc.

- *Molecular chemistry, because of the nature of its reaction media composition and kinetics, is ahead of other disciplines in understanding the intermediate steps in chemical reactions (regarding dynamical features of reaction mechanisms).* This is particularly the case regarding the process of choosing starting compounds vis-à-vis their structure, composition, and morphology, with the purpose of orienting the reaction towards the desired compound.

It is important to improve the properties of new and existing materials through the *interplay among the structure, the composition, the mastery of the defects, and the morphology*. The purpose here is to confer new and existing materials with specific properties in relation to certain demands, such as those imposed by the disciplines of electric, electronic, catalytic, civil or mechanical engineering as well as in relation to the production of equipment based on optical, optoelectronic, electric, or magnetic components.

We need to *characterize with an ever-increasing fineness the chemical, structural, and physical properties of the pure compounds and their association within heterogeneous systems* (bulk and interfaces in wide ranges of operating conditions). It will be a question of extending and deepening the understanding of the existing relationships among the chemical composition, the nano- and microscale molecular structures, and their properties. This particularly concerns granular materials, porous media and, in a general way, those materials for which the surface/volume ratio is very high. One spin-off of new synthesis processes and the means in which materials are characterized at the nanoscale (interfaces, nanoparticles, aggregates, etc.) is the development of a nanochemistry and a nanophysics, which will lead nanotechnologies. The recent emergence of carbon and boron nitride nanostructures is a promising example.

It is important to intensify the efforts in *numerical simulations and modelling* for the prediction of both structures and properties. Simulation, in addition to experiment and theory, appears to be a third way to solve problems in physics. The most obvious aspect of simulation is its capacity to provide quantitative answers in complex physical and/or geometrical situations for which the analytical tools are no longer operational. While numerical simulations can also be used to conceive model designs, it only accounts for certain aspects of the physical reality. Numerical simulations might lead to successful predictions of (physical) behaviours, at least qualitatively. Solid-state chemistry and materials science's structures-properties relationship that implements micro/macroscale changes can be modelled and treated with the help of numerical simulation. Particular emphasis should be given to the following in terms of nanostructure modelling:

- Modern computational techniques of the calculation of band structures by self-consistent methods (DFT-based), including volume, surface, interfaces, etc.
- A combination of the calculation of density of states, statistical physics, and numerical methods (Monte Carlo, molecular dynamics, etc.).

Finally, we must compare the respective outcomes of characterization methods and calculations in order to permit a qualitative and quantitative study of the chemical bond in solids (charge transfers, band structures, etc.). What are the most appropriate methods to study the ionocovalent solid?

1.4.3. Molecular Inorganic Chemistry – New Routes to Hybrid Materials (Inorganic and Inorganic-Organic)

Looking toward the 21st century, the nanosciences will be, like biology, one of the fields that will contribute to a high level of scientific and technological development. At the beginning of this new era, *molecular approaches of solid state chemistry and nanochemistry* have already reached a high level of sophistication. Today we are close to mastering the synthesis of many organic ligands or molecules, coordination metal complexes, functional organo- or functional metalo-organic precursors with functional nanobuilding units (NBUs; or NBBs for nanobuilding blocks) carrying magnetic, electrical, optical, or catalytic properties.

A large amount of research has been undertaken to obtain organic templates (surfactants, dendrimers, organogelators, polymers, block copolymers, multifunctional organic

connectors, biopolymers, etc.) and to understand their physicochemical properties. Indeed, many research programmes or research actions have been devoted to Organized Molecular Systems (OMS) or Organized Polymeric Systems (OPS).

(a) State of the art

Nowadays, chemists can practically tailor any molecular species – from molecules to clusters or even to nanosized particles, nanolamellar compounds, or nanotubes. Clusters are mainly being used as model compounds, while nano-objects are common in the more applied research fields.

The various characteristics of the soft chemistry-based process (molecular or NBB precursors, organic or aqueous solvents, low processing temperatures, and processing versatility of the colloidal state) allow the mixing of inorganic, organic, and bio components at the nanometric scale in virtually any ratio, leading to the so-called hybrid organic-inorganic nanocomposites. An extraordinary amount of research has appeared in the field of hybrid materials, indicating the growing interest of chemists, physicists, and materials researchers to fully exploit this technical opportunity for creating materials and devices benefiting the best of the three realms: inorganic, organic, and biological. Because of their high versatility, which offers a wide range of possibilities in terms of chemical and physical properties and shaping, hybrid nanocomposites present the best means for both facilitation of integration and device miniaturization.

Moreover, hybrid materials can possibly be used directly as innovative advanced materials or as precursors of novel inorganic solids, opening the way to promising applications in many fields, including optics, electronics, ionics, mechanics, membranes, functional and protective coatings, catalysis, sensors, and biology.

In the United States and Japan, scientific production in molecular inorganic chemistry is more important than it is in Europe. This is probably caused by a more empirical and systematic approach to the research by the U.S. and Japan. However, in Europe chemists working in this research field have a better understanding of the mechanisms involved in the formation of materials and, consequently, a better control of chemical reactions and a good reproducibility of their results. This European approach, which is based on outstanding, comprehensive fundamental research in complex systems, must be encouraged.

(b) Future visions and expected breakthroughs

New molecular compounds and innovative NBBs will, of course, appear in the near future. The challenges of this new century are related to the smart use of these highly sophisticated chemical tools for research in biology and/or materials science.

The nanostructure, degree of organization, and properties that can be obtained for hybrid materials certainly depend on the chemical nature of their components, but they also rely on the synergy between these components. Thus, a key point for the design of new hybrids is the tuning of the nature, extent, and accessibility of the inner interfaces.

A suitable method for a better defining of inorganic components and hybrid interfaces exists in the use of perfectly calibrated preformed objects (such as clusters, nanoparticles, or nanolayered compounds) that keep their integrity in the final material. The variety found in nanobuilding blocks (nature, structure, and functionality) and links allows to build an amazing range of different architectures and organic-inorganic interfaces associated with different assembling strategies. The confinement of highly dispersed nanobuilding blocks in hybrid or inorganic matrices, or the organization of NBBs on textured substrates, could provide larger concentrations of active dots and better-defined systems, and could help to avoid coalescence into larger ill-defined aggregates while keeping or enhancing specific magnetic, optical, electrochemical, chemical, and catalytic properties into the nanostructured hybrid materials.

Because there now exists a basic understanding of the role of molecular and supramolecular interactions between template molecules and hybrid or inorganic-based networks, templated growth-based processes using organic molecules and macromolecules as structure-directing agents can now allow the construction of complex architectures. These strategies are used by researchers, who try, somewhat naively, to mimic the growth processes occurring in biomineralization.

Strategies combining the nanobuilding blocks (NBU or NBB) approach with the use of organic templates that self-assemble and allow to control the assembling step have to be more developed. This combination between the "nanobuilding block approach" and "templated assembling approach" will be of paramount importance in exploring the possibilities for building hierarchically organized materials, particularly in terms of structure and functions.

In the near future, original materials will be designed through the synthesis of new hybrid nanosynthons (hybridons) selectively tagged with complementary connectiv-

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ities, allowing the coding of hybrid assemblies presenting a spatial ordering at different length scales. Hybridons carrying chirality and/or dis-symmetry (Janus-type NBBs) and complementary functionalities will open new pathways for the synthesis of these materials.

With skilled chemists setting original pathways in materials processing, numerous scientific breakthroughs can be expected in this field. The synergy between chemistry and chemical engineering will permit an access to materials having complex structures that allow a high degree of integration. In particular, a synthesis obtained through the construction of materials by the simultaneous use of self-assembling processes and morphosynthesis (exploiting chemical transformation in spatially restricted reaction fields) coupled with the use of external forces (such as gravity, electrical and magnetic fields, and mechanical stress) or even through the use of strong compositional flux variations of reagents during synthesis (open systems) will allow the generation of innovative hierarchical structures.

Chemical strategies offered by such coupled processes (self assembly + morphosynthesis + external solicitations) allow, through an intelligent and tuned coding, the development of a new vectorial chemistry that is able to direct the assembling of a large variety of structurally well-defined nano-objects into complex architectures. Multiscale-structured hybrids or inorganic networks (from nanometre to millimetre) will open a land of opportunities for the design of new materials. Could these new synthesis strategies allow us to dream of a future where it is possible to build intelligent advanced materials that respond to external stimuli, adapt to their environment, and self-replicate, self-repair, or self-destroy at the end of their useful life cycle ?

(c) Research needs

Such an innovative field of research will strongly benefit and become more mature through developments and advances in the following areas:

- Better knowledge of soft chemistry routes from precursors to materials.
- Improved knowledge of interfacial chemistry and physicochemistry of nanocomposites.
- Study of phase diagrams of hybrid composites.
- Better knowledge of organized-matter soft chemistry.
- Study of order/disorder transition in hybrid nanosystems.
- Relation between order and disorder and a given property of the hybrid (e.g., mechanical).
- Better knowledge of reactivity, stability, and connectivity of NBBs.
- Synthesis of new nano-objects and nanohybrids with tuned functionalities, with dissymmetric functionalities or carrying chirality.
- Synthesis of nanoparticles with a controlled surface chemistry, adjustable size, sharp- sized distribution, and redispersability.
- Clean and environment friendly process.
- Development of 2-D hybrid networks, lamellar, films, etc.
- Development of bio-inspired materials.
- Hybrid materials having modulable mechanical properties.
- Development of materials that can adapt their response to external stimuli (e.g., pH, solvent, light, external fields, temperature).
- Smart functional coatings (highly hydrophobic or highly hydrophilic, protective, anti-corrosion, anti-scratch, etc.).
- Intelligent, hierarchically structured membranes that can couple separation and catalytic processes.
- New adsorbants.
- Hybrids for photonics having photochromic, emission, absorption, lasing, nonlinear optical, electroluminescent properties for designing new sensors, optical memories, lasers, and display devices.
- Development of biohybrids that will benefit fields, such as biosensors, imaging, immunoassays, vectorization with controlled release, hybrids allowing better compaction and thus transport of ADN, protection of fragile biocomponents, etc.

1.4.4. Inorganic Amorphous Solids – Glasses

Because of their thermodynamic status as frozen liquids, glasses occupy a peculiar position in the general classification of materials science. Above the so-called glass transition temperature, these metastable but extraordinary solids exhibit temperature-dependent plasticity that allows industrially controlled operations such as blowing, fibering, and moulding. Under the same conditions, these metastable compounds tend to come back to equilibrium in nucleating microcrystals or molecules, forming vitroceramics or foaming glasses. This situation could enhance some properties, such as mechanical strength, but could also be detrimental to others, such as light propagation in optics. The easy glass-forming ability is the privilege of some oxide families, such as the silicates, which allow us to prepare such sophisticated objects as optical fibres for telecommunication and low-cost products for the automobile or building industry. From a purely marketing or public visibility point of view, these materials are the driving force of the research and glass industries.

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Curiously, these paradoxical materials could be synthesized at a mass-production level in large homogeneous pieces, but their structures at a nanometre scale are still obscure. Recent programmes have liberated the exotic vitreous materials from their stereotypical research niches through the development of new nonoxide glass compositions that offer optical properties not permitted by traditional oxide glasses. In addition to benefiting the optoelectronic industry by creating new materials for original functions and devices, these new glasses allow a better understanding of the concept of liquid polymerization and glass formation.

We are in danger of being mired in Byzantine and esoteric discussions about the nature of glass, and not gaining significant knowledge of the structure of the actual material. It must be accepted that basic research should be driven by specific targets that lead to actual applications. This offers the advantage of stimulating creativity, especially among the next generation of researchers, permitting a means for objective evaluation as well as raising the interest of the industrial community.

(a) State of the art

Research on vitreous materials is by essence rather empirical and time and labor intensive, but the investment is justified by the unique characteristics (in terms of homogeneity, volume, shaping, and purity) of the products. In the last few decades, basic research in the field has been driven by pure academic curiosity or technological need, and in both cases, with great success. The following domains have been especially prolific:

i) *Glasses for photonics* is the sector having the most spectacular results. Driven by telecommunication needs, outstanding results have been obtained in the preparation of ultrapure silica glass for fibres in such a way that the theoretical limit in transparency has been reached in the all-telecom window. Also, the development of rare earth doped glasses for optical amplification, as well as the possibility of local modification of the glass refractive index under laser illumination, is revolutionary. The association of Bragg gratings writing, optical amplification, and planar waveguide integrated optics on glass to split and recombine the optical signal has been proved to be the key factor in the worldwide success of Dense Wavelength Division Multiplexing (DWDM) for high-capacity information transmission. Other lanthanides than erbium are needed to expand the all-telecom window, but their efficiency will be dependent on new glass matrices that have low phonon energy. Some preliminary positive results have already been obtained with exotic materials such as fluoride- and chalcogenide-based glasses.

Another important research effort has been the development of glasses having nonlinear properties for optical fast switching second harmonic generation and for local mastery of the refractive index under light of electric field exposition. This newborn field has fascinated both the academic and industrial community.

New chalcogen-based glasses having excellent transparency in the infrared range, particularly in the two atmospheric windows, are in the pioneer stage of development. They will be used in the moulding of low-cost IR optics for cameras or night-vision systems to assist drivers, fire fighters, police officers, and others operating under conditions of poor visibility.

The mastery of glass fibering is critical not only for telecommunications but also for the development of optical fibre sensors operating in the visible, but also in the infrared light range, which will permit the *in situ* observation and collection of precious information on chemical and biological processes.

ii) *Glass surfaces are a permanent subject of investigation*. This is necessary for a better understanding of basic problems such as corrosion mechanisms, fractures propagation, ionic exchange for glass strengthening, and antireflective or reflective coatings for improving the thermal characteristics of window glasses. The controlled modification of the glass surface refractive index by implantation ionic exchange, and thermal or sputtering deposition has also received a great deal of attention for its possibilities in planar or channel optical wave-guide development. All of these technologically oriented objectives need to be supported by a strong mastery of the fundamental concepts of chemical bonds, diffusion, relaxation, local structures and mechanical stress. In connection with the previous topic of glass photonics, the field of glass interfacing with other materials is also very important. Glasses are almost everywhere and can be in contact with many different compounds, ranging from metals to biological tissues. This observation has generated creative works on bio-glasses and their interface with bones as well as interface mechanisms in glass/metal welding.

Important but limited contributions have also been published on composite materials involving interfacial problems between glasses and polymers that are both in the vitreous state and that raise both fundamental and technological interest. The control of the glass-to-crystal transformation has permitted the mass production of vitroceramics, composite materials having exceptional mechanical properties. This is a good example of industrial fertilization by basic research.

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iii) *The last decade has also been characterized by the discovery of new glass-forming systems* belonging to a wide-range of chemical families, from the chalcogenides, to the fluoride nitrides, to original metallic combinations, (e.g., Zr/Cu based). These new glasses have reached a maturity that has justified the development of prototypical industrial products, but the underlying reasons for glass formation and the criteria for stability are still unknown.

iv) The same period has also seen the emergence of mathematical simulation approaches as well as access to powerful instrumentation based on neutrons, X-rays, synchrotron radiation, and variable spectroscopies such as Mössbauer, NMR, and Raman. This situation has permitted the opening of a small window into glass structures, which for the most part still remain a mystery especially at a medium-range order.

v) In general, glass research in Europe is characterized by a parcelling out of programmes and funding such that the research is always driven by short-term demands. The consequence is that there is never enough time to reach significant progress. On the other hand, in Japan, the policy is quite different. Through Exploratory Research for Advanced Technology (ERATO), long-term programmes are supported. For instance, the HIRAO Active Glass Project has been launched for at least five years, allowing creative research in such areas as new glass discovery and physical properties, and also providing a permanent structure for transfer of research to industrial applications. In the U.S. the glass community is well identified through the glass division of the American Ceramic Society, which provides a permanent forum for exchange with many industries, ranging from buildings to art to telecom. This situation does not exist in Europe, which needs to be strongly encouraged to fertilize the cross-exchanges between basic research and application in the glass field. This is especially important because the field is always evolving, with such fast-growing markets as telecommunications.

(b) Future visions and expected breakthroughs

It is now clear that glasses, when compared to other materials, offer the unrivalled advantages of easy shaping, homogeneity, and large-volume production. However, the price paid for these superiorities is the necessity for perfect control of the glass-forming conditions, a precise ratio in the glass-to-crystal balance, and mastery of all kinds of perturbations, which usually arise at the surface. Once these problems are solved, new low phonon energy glasses belonging to nonconventional families such as the halides, chalcogenides, and others will play a key role in the future of *photonics*.

It is critical to encourage *a priori* research on new chemical compositions instead of merely following the demands of the technology. New materials will automatically generate interest in the immense field of photonics and will also generate new ideas for applications. The creation of new glasses, with the periodic chart as an inspiration, will assure that this science is not merely at the service of technology. For example, in the past, glasses were not identified as their own EC materials research programme. Instead, they were considered to be a subprogramme of telecom or another area. *Photonics* will continue to be the main partner of new glasses through the huge market of telecom, but will also partner with glasses because of the growing need of optical sensors. Important breakthroughs are expected in new glasses, particularly in the design of glass-integrated devices, including main optical functions such as amplification, splitting, or filtering. The understanding and control of phenomena such as photo-refractivity and electrical poling will be necessary. Obviously, new emerging fields such as bioglasses or composite glass/polymer materials will find a significant amount of support for development due to a strong industrial and medical demand.

The materials scientists cannot be proud of the results obtained in the field of batteries and *energy storage* in general. Glasses have received very little attention in this domain, and they must be reconsidered as potential materials for cationic or anionic conductive membranes, especially when considered in their plastic regime. Future breakthroughs in this critical field will come from looking at glasses as viscous liquids. Many development lines are also expected, particularly for films in association and complex compositions in order to obtain *unwetable, self-cleaning, and unbreakable glasses.*

(c) Research needs

The number one priority in the frame of a long-term basic programme is clearly *to encourage the creation of new vitreous materials*. This includes the discovery of new, original glass families that correspond to the control of subtle interactions among a complicated ensemble of atoms, as well as the mastery of the industrial compositions from a chemical and chemical-bonding point of view. In order to understand the deep-formation mechanism, many powerful instruments are available for structural investigations, but they need to be restricted to select types of novel glasses.

The interactions of light with glass is also a priority and corresponds to scientific interests as different as photorefractivity, ultra-transparency, broad band transmission from deep UV to far IR, non-linearity, fluorescence, pho-

tochromism, optical sensors, etc... Glasses for telecom will certainly be supported from the telecom side, but optical glasses for sensors, lasers, and IR technology which have been neglected to much until now need to be encouraged to put the European industry at the same level as in the U.S.

Research programmes on glass surface need also to be reinforced for a better understanding of mechanical, optical properties, interfacial problems with other materials. This include for instance anti-reflecting or hard coatings and all kinds of glasses. Also funding must be saved for exploratory projects corresponding to specific niches such as bioglasses or electrochemical glasses for batteries and other exotic applications.

The investigation of *glass formation mechanisms* from the molten salts and also through sol-gel or gaseous phases must be considered as long-term projects that will generate new ideas for the access to new materials.

The glass surface also needs to be the subject of special attention because it corresponds to the place that interacts with the outside and where defects or anomalies propagate into the bulk. A good knowledge of *surface chemistry* could also help the industry control chemical or mechanochemical polishing.

From a purely fundamental viewpoint, efforts should be pursued in the *understanding of the vitreous transition and the modelling of glass structure*.

1.5. Soft Materials and Polymers: The Rise and Decline of Polymer Science & Technology in Europe

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Macromolecular Sciences and Polymer Technology at Crossroads?

Europe is facing a major restructuring of its polymer producing industry with many mergers and a strong decrease in long-term corporate research within many companies. In combination with a strong decrease in the enrollment of students in physical sciences in the last decade, the future of polymer science & technology in Europe might be at stake. In this article, the situation is analysed with references to the other invited authors in this special Magazine of the European Polymer Federation (EPF).

Europe has been the cradle for Polymer Science & Technology. At the very start of the last century, Baekeland synthesized the first fully synthetic material in Gent (B). Polymer Science was founded in the 1920s when Staudinger postulated its concept of a polymer chain, consisting of covalently bonded monomeric units. The birth of the polymer (plastic) industry took off after World War II and was boosted by the invention of Ziegler and Natta's heterogeneous catalyst systems, in the mid 1950s, enabling the production of (linear) polyethylenes and stereoregular polypropylenes at relatively low pressures and temperatures.

In retrospect, the invention of the Ziegler/Natta catalyst systems and the implementation by industry in direct production is the paradigm of co-operation between academia/governmental institutes with industry. In the 1950s within 5 years, Montecatini in close co-operation with the university of Milano (Natta c.s.), were able to develop a commercial process to produce 'isotactic' polypropylene [1]. The further development of more efficient catalyst systems (by a factor of more than 10.000!) by Montecatini, Montedison, Montell (now Basell) shows the strength of industrial R&D, viz. optimization to the extreme. The current production of 30 million tonnes of i-PP per annum at a cost of around 0.5 Euro/kg, viz. 6 kg/capita in the world, shows the tremendous impact of the invention by Natta and Ziegler.

In the 1980s, the novel homogeneous single-site (metallocene-based) catalyst for the production of polyolefins, with enhanced control over the molecular structure, were also rooted in academia in Europe (Kaminsky/Hamburg; Brintzinger/Konstanz). The impact on the industrial polymer production is not yet clear but expectations are running high.

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The area of synthetic polymers is usually divided into 3 sectors, viz. commodity plastics, engineering plastics, and speciality polymers. At the end of the 1970s, the area of commodity plastics was considered to be rather mature, comparable to the steel industry (a few standard grades produced in high volumes at low costs) whereas the future was foreseen in the area of speciality polymeric materials and products. However, industry has developed numerous grades based, e.g., on supported Ziegler/Natta catalysts and copolymerization technologies. With the development of the novel metallocene-based single site catalysts, in principle, even more control is gained over the molecular architecture and novel copolymer grades and new polymer types could be produced, such as syndiotactic polypropylenes and polystyrenes. Consequently, the term commodity plastics is not applicable anymore. The name polyethylene, the polymer produced in the largest amount (close to 50 million tonnes/annum), is in fact only generic and represents a family of numerous grades, some of which can be considered to be specialities.

The 1980s can be considered as the decade of 'High-Chem' in view of huge research efforts, both in industry and academia, to search for ultimate performance for polymers as construction materials (liquid-crystalline-polymers; high-performance fibres and light-weight composites; novel polymer blends with synergistic properties compared with the constituents etc.). Moreover, a new dimension was added to polymers: functionality. Examples are polymeric materials that conduct electricity (Heeger, Mc Diarmid and Sirakawa, Nobel Prize for Chemistry in 2000) were discovered and polymers that emit light (poly-LEDs) upon applying a voltage (Friend c.s. Cambridge).

Despite the major research efforts during the last two decades, the volume of speciality (functional) polymers, engineered on a molecular scale for specific applications did not increase in volume, it is still below 1 vol% despite high expectations. This low number seems not only to apply to the production volume but also to the production value. Nevertheless, speciality/functional polymeric materials and products are indispensable nowadays in many applications, notably in the ICT and medical technology. Companies such as Philips take a serious effort to make use of speciality polymers, for example in display technologies.

In retrospect, synthetic polymers are typically materials of the 20th century in terms of birth, growth and innovations and Europe has played a key-role in these developments, often in close concert between industry and academia. At the turn of the century, however, drastic changes occurred which could have a profound and adverse effect on the future of Polymer Science & Technology in Europe:

- In the last decade, some leading polymer producing companies in Europe, with the prime example of Hoechst, decided that their future business is not focused anymore on polymers (plastics) but on 'Life-Science'. The highly cyclical petrochemical industry with unpredictable profit is incompatible with the new trend of share holders value.
- Major mergers occurred, e.g. Petrofina-Elf-Total, Basell (Shell/Montell/BASF and the former Hoechst parts Elenea and Targor) and BP/Amoco, a process that appears not be completed up to now and takes place in the U.S. as well (DOW/UCC; Exxon/Mobile).
- In general, corporate research activities within the petrochemical industry declined, or were even terminated (Akzo Nobel) including potential promising developments, e.g., the polyketone (co)polymers, Carilon® by Shell.

The driving force for the events mentioned above is cost reduction which can be realized by increasing the scale of operations, not only in terms of the size of the newly merged companies (sales) but also in terms of plant capacities. Currently, up to 600 kilotons/annum polypropylene plants are under construction. Combined with the trend of recycling in the automotive industry, the future focus will be on simple, cheap polymers, with a preference to use monomaterials instead of sophisticated blends, one of the major research activities in the 1980s with thousands of patent applications per year (may be this statement is for the moment only applicable for blends produced in reactors and not for sophisticated blends produced by mixing). The strong growth of the cheap and versatile polymer polypropylene, reinforced with fibres and/or particulate fillers, in the past decades, penetrating in the area of engineering plastics (automotive) demonstrates this trend.

Considering the present situation, the title of this article seems to be justified. The key question for the future is whether the polymer manufacturing base, after consolidation, will stay in Europe or will move out of Europe in due time, e.g., upstream to the oil wells in the Middle-East or even more eastbound, to China .

A parallel, but even more important question, is whether there will be a market in Europe for specific polymer grades with a high(er) added value than the standard bulk grades, produced by dedicated plants close to the customer (customer intimacy).

The gap between the petrochemical industry, with the focus on consolidation and a strong increase in the scale of operation (plants producing up to 600 kilotons/annum), vs. the world of speciality/functional polymers in various

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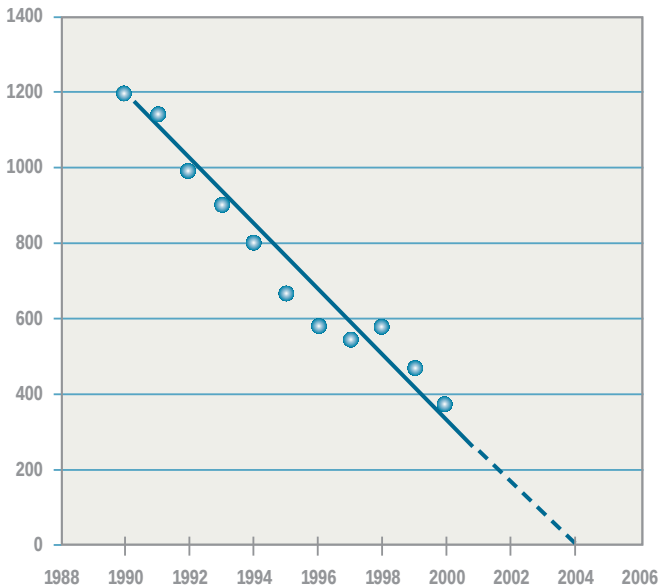
high-tech applications, on a scale of kilograms, is apparently widening. Producing specific grades in large capacity plants is contradictory.

The gap could be bridged, in an optimistic future scenario, by stimulating young scientists and engineers to become more entrepreneurial and to start small-sized companies for development and initially low volume production of speciality polymers, which eventually can be taken over by well-established companies eagerly looking around for proven novel technologies which are not generated so easy anymore in-house due to their extensive trimming of corporate, long-term, research. The current trend of outsourcing long-term research by industry to academia and government institutes could well catalyze this scenario. On a national scale there have been several initiatives to promote co-operation between academia and industry, e.g., the IRC's in the UK, the Danish Polymer Centre and recently the Dutch Polymer Institute (DPI) where the research agenda is set in a strategic alliance between universities and industry (for more info visit: www.polymers.nl).

The question to be answered is whether in the present climate of a unifying Europe the dedicated (young) workforce can be found and motivated to take up the challenge of scientific entrepreneurs in the area of polymeric materials. A lot of challenging jobs have been lost in the petrochemical industry, due to trimming of corporate research and mergers. As a consequence (and this is the personal opinion of the author), the enrollment of students in hard physical sciences such as chemistry and physics has decreased to very low numbers. Fig. 1.10 shows the enrollment of students in chemistry & chemical engineering in The Netherlands in the last decade, from 1200 students in 1990 to less than 400 students in the year 2000. Similar data can be observed coming from Germany, France, Belgium and the UK. These numbers have to be compared with a developing country such as India where the five major IIT's (Indian Institute of Technology's) can select each year their 2000 new students from over 200.000 applicants. The recent move of GE corporate research to Bangalore (India), the new John Welch corporate research centre, to be followed by others (Exxon?) is an indication that in some board rooms the conclusion has already been made: the future of materials sciences, including polymer science goes eastbound ? Looking Eeast in Europe, our colleagues within the European Polymer Federation (EPF) tell us that despite the often eroded infrastructure, still motivated (young) people pursue a scientific education.

Fig. 1.10. Enrollment of students in chemistry and chemical engineering in the Netherlands.



Within the EPF, the national representatives of the member states concluded that the strong decrease in the enrollment in physical sciences, seemingly in line with a decrease in industrial long-term research, is considered to be the major topic of concern where action is needed. The industry has been invited to discuss this issue and to make an action plan, for example during the EPF meeting in Smolenice (Bratislava) in October 2000 and again during the Europolymer Congress, July 15-20, 2001 in Eindhoven (www.europolymer.org). The future of Polymer Science & Technology in Europe is at stake.

In view of all the expertise in Europe, combined with a strong tradition in polymer science, embedded in a strong scientific culture, new ways to stimulate further development of polymer science & technology have to be found. In a unifying Europe, national laboratories should be linked into a virtual institute, stimulated by the EU. Communication is key and the new internet-journal 'e-polymers' could function as the platform for exchange of ideas and act as a discussion platform in Europe. Education beyond traditional disciplinary methods at European level could stimulate research in new areas. Many more ideas are needed to shape the future of polymer research but for that purpose discussion is needed among the stakeholders.

No doubt that synthetic polymers will continue their growth but challenging problems will be encountered during this century. At present, only 5% of the world oil supply is used to make synthetic polymers. If, however, countries in Asia etc. will continue their growth, aiming to reach the level of the industrialized world (and they should), the production volume of polymers, and consequently, the use of oil for this purpose will grow with a factor of ten, in competition with oil needed for energy. Needless to say that

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macromolecular sciences, including biotechnology, and polymer technology are coming soon at crossroads to ensure a sustainable growth of synthetic materials, increasingly based on renewable feedstock.

Combining the world of biotechnology, macromolecular sciences and polymer chemistry/technology, focusing on concrete research targets for the (near) future, might well be the answer to attract and motivate talented young students. Many departments already realized that by simply changing the name from materials into biomaterials, had a very positive effect on the enrollment, also on women. Once 'on board' talented young students will realize that polymer science, the science of making and manipulating long chain molecules, is a highly interesting field independent whether these molecules are of synthetic or natural origin. There are major challenges ahead of us to further exploit the intrinsic possibilities of long chain molecules ranging from the focus on ultimate performance in 1-D, 2-D or 3-D(imensions), via structuring polymer molecules in devices (displays, plastic electronics) to mimicking nature in tissue engineering and other advanced biomedical applications.

May Europe take the lead in these future developments!

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1.6. Soft Materials and Polymers: Strategies for Future Areas of Basic Materials Science

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1.6.1. Introduction

Soft materials are characterized by weak but nevertheless long-range interactions among the molecular or supramolecular constituents. These interactions lead to the formation of static and frequently also dynamic structures of hierarchical nature and physical properties which depend largely on cooperative interactions on various length and time scales. The industrially most relevant class of materials in this context are *synthetic polymers.* Moreover, *all life forms* are built and organized of soft biogenic materials; this includes connective *tissue, bone* and similar materials from which the *skeleton or exoskeleton* are formed, the structural elements of cells (cell membrane and scaffolds), *carbohydrate*-based materials in plants and produced by them (e.g. cellulose, starch). The area also includes materials on which advanced technologies are based like *colloids, liquid crystals, composite materials* (fibre-reinforced plastics), and *photoresist* materials as they are necessary to create the hardware of information technology.

Most of the soft materials are based on organic molecules or macromolecules ("polymers"). It is irrelevant for their physical behaviour whether they are synthetic or biogenic.

In the class of *colloids* which consists of weakly interacting nano- or microparticles in a fluid medium we find inorganic materials as well, but even there, interaction with organic *surfactants* is frequently decisive to obtain stable or metastable situations. Thus, *surfactants* are summarized as well in the context of soft materials. The modification of the surface of common materials and of constructions or parts made of common materials is prerequisite to modern technology. The modification by, e.g., coatings serves to protect the materials against *corrosion (coatings) or abrasion (tribology)*, it allows for deposition of information *(printing technology)* or distinction *(advertising, coloration)* and it also helps to connect parts of different quality and function *(adhesives)*.

1.6.2. Polymers: State of the Art

The production, modification, and processing of polymers is most important to European industry. The world production of polymers has now by far exceeded the production of steel (by weight) and is close to 180 million tons in the year of 2000. Europe has a share of ca. 28

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percent (50 million tons) equivalent to a production value of ca. 100 billion €.

Processing of plastics as distinguished from the production is an industry of own character and constituency. While the production of polymers is dominated worldwide and even more so in Europe by very few big players – the chemical industry – , the processing industry is characterized by thousands of small and middle sized industries (e.g. in Germany one finds ca. 2.500 enterprises with a total of ca. 220.000 employees). About 60 percent of the production of polymer materials is used to supply *structural materials* to the market. 40 percent are produced to serve as *functional materials.*

(a) Structural polymers

Most of the polymers produced as structural materials ("standard plastics") are based on polyolefines (polyethylene, polypropylene, and similar hydrocarbon polymers and copolymers). The final application is found in the areas of *packaging* (41 %), *construction* of buildings (20 %), *electric insulations* (9 %), *automobile parts* (7 %), *agriculture* (2 %) and miscellaneous (21 %). The application of plastics to substitute more conventional materials (e.g. metals, glass, ceramics in the packaging industries) or to develop *new technologies* (e.g. audio/video discs) is innovative and a constant source of industrial evolution. We also find substitution of more expensive "specialty" polymers by new generations of "commodity" polymers. This relates to the constant improvement of the processing properties and physical characteristics of polyolefines by the invention and adaption of *novel catalysts* in the polymerization processes. The new structural variations at the level of the molecular architecture lead to a constant evolution of the properties in application.

Innovation in, e.g., the food packaging industries by availability of new or improved polymer based materials is essential to the development of the distribution and storage systems in Europe and assists in the restructuring and development of the agricultural regions. The large-scale replacement of glass by polyester-based materials ("PET") for fluid containers in the soft-drink industry is another example. The initial problem of plastics waste disposal has been solved in recent years by a combination of legal actions and economically viable collection and redistribution systems.

It is necessary to mention that speciality polymers have a firm place in modern industry and have frequently the character of an *enabling technology*. An example is the production, application, and constant evolution towards improved performance of epoxyresins, a class of polymers which serves as insulation and packaging material in the *electric/electronic industries.* It is basic to modern electronic industries.

(b) Functional polymers

Polymers produced as functional materials serve in a multitude of applications as additives, processing aids, adhesives, coatings, viscosity regulators, lubricants, and many more. They are found in cosmetics and pharmaceutics, in all kinds of semi-prepared foods, in printing inks and paints, as superabsorbers in hygienic products and in the processing of ceramics ("binders") and concrete, as flocculants in waste-water treatment and as adhesive in the hardware production of electronic equipment, just to mention a few.

New developments of functional polymers have had revolutionary effects on the industries in which they found application in that they provided the enabling technological base to novel or improved production systems. Moreover in many cases totally new applications became available. An example is the now widespread use of superabsorbers in personal care products, which in itself created a totally new industry with novel product lines. The biomedical application of polymers needs also to be mentioned here. Polymers play an increasing role as implants, in dentistry, in the surgery of connective tissue and arteries as well as in general medical technology. It constitutes a large market of its own right and of interdisciplinary research activities.

One also needs to mention that the provision of novel functional materials has also large repercussions on the machine and production line industries. A good example is the printing machine industry. Progress in this industry depends largely on the provision of new printing inks optimized for high speed printing processes – largely a "polymer problem". The same is true for "laser-printing technics", the speed of which depends largely on the polymer based printout process.

1.6.3. Research Topics

A survey among the European Industries leading in polymer production in the years 1998/99 gave the following high-priority targets for research devoted to polymers:

- *Emulsion polymerization:* find ways to go from batch type reaction to continuos reaction; this would need the development of new, most probably polymeric surfactants; the stability of emulsions and dispersions needs to be improved, the aging and film formation need to be better controlled; this would have enormous impacts on the coatings and adhesives industries:

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- Enhanced efforts in the finding and evolution of *catalysts for olefine polymerization*, with emphasis on metallocene based catalysts. Here, copolymerization, heterogeneous catalysts to be subject to fluidized bed polymerization processes, synthesis of elastomers by metalcatalyzed processes are key targets.

- Better data on *reaction kinetics* and on *transport phenomena* in multiple systems would greatly help to improve the large scale production of polymer materials.

- The formation and processing of *particulate systems* (highly filled polymers, coating formulations, printing inks etc.) which includes understanding of the growth kinetics of particles and surface grafted particles would help to advance exisiting technologies significantly.

- *"Solvent-free" polymerization* processes are desired to reduce environmental hazards and reduce the costs of polymer production.

- *Polymerization in aqueous media*, water born polymers and water based coatings would also reduce environmental hazards of present technologies.

- *"Reactive extrusion"*, that is creating application targeted products in the processing step would enhance the market situation of the small- and middle-sized processing industry.

- A further development of *analytical methods* and quantitative *methods of characterization* of structure and performance of polymer materials is highly desired; among these, *in situ* technics of determination of the molar mass distribution have the highest priority; equally important is the development of fast and precise methods to determine the structure of branched, hyperbranched, and crosslinked systems. The analytical characterization of particulate systems and of dispersions needs to be improved.

Most of the polymer materials in present days technologies exhibit part of their function in contact with the outside world, that is by their surface properties; key words which need attention in research in the immediate future are therefore:

- *Adhesion:* understanding and improvement of the mechanisms of adhesion and failure of adhesives, prevention of adhesion by surface modification, development of "tacky" polymers (time/ temperature/ pressure-dependent adhesive processes), general studies on wetting/ dewetting processes, adhesion between living systems (cells) and polymers, "bioadhesives".

- *Polymers for medical applications:* polymers designed to act as implants, polymer-tissue and polymer-cell interactions, aging of polymers exposed to biosystems, materials for artificial organs, materials in pharmaceutical and medical technology. High-purity polymers, membranes, membrane materials for hemodialysis, polymers in medical diagnosis.

- *Polymers for advanced technology:* polymers as storage media of information (audio/videodiscs); photoresists and related materials necessary to produce advanced electronics hardware; polymers in display technologies: alignment layers, polarizers in LCD's, electroluminescent polymers for OLED's; separator membranes and ion-conducting binders in power supplies (fuel cells, Li-ion batteries) for portable or mobile applications.

- *Computational techniques:* The advance of theoretical understanding of the behaviour of polymer materials opens the way to relate details of the molecular structure and changes thereof to the performance in processing and application. Large scale computing using dedicated software is necessary. However, progress in the simulation of expected behaviour based on molecular architecture would greatly speed up the research process in the production of polymers, thereby giving European industry a lead over its competitors. Europe is presently leading in computational techniques in this field but its results need to be transferred to industry and – at the same time – the methods of simulation have to be improved with regards to the full spectrum of application of polymers in practice.

1.6.4. Future Perspectives of Basic Research in Soft Materials and Polymers

The properties and the application of "soft materials" (polymers, biopolymers, composites, liquid crystals, surfactants) are based on weak but long-range interactions among the molecular constituents. It is poorly understood how and why these interactions lead to hierarchical structures and in most cases time-dependent physical and engineering properties. The controlled achievement of the architectures is key to applications.

(a) Polymer synthesis

The synthesis of commodity or engineering polymers is dominated by the impact of finding new catalysts for improved polymerization processes. The need to find novel principles of catalysis to be used in already existing large-scale polymer production facilities is unrivalled. Moreover,

tailoring the molecular structure, e.g., the mass distribution of the chain length, the stereochemical microstructure and copolymer composition to enhance the processing and performance of polymers is key to further growth.

The synthesis of speciality polymers is geared towards functional purposes and to polymers as enabling materials. Novel polymers are key in the development of electro-optical devices in modern communication (e.g. light emitting diodes, displays, sensors, batteries; see Fig. 1.11) and in biomedical applications (artificial lenses, joints, skin, arteries etc.)

(b) Supramolecular structures

The properties of polymers depend on structural organisation at various length scales. The relation between molecular structure, conditions of processing and principles of self-organization are largely unknown or only empirical rules do exist. Further progress in exploiting the intrinsic properties of polymers thus depends on gaining more insights how to control the interactions between the constituent macromolecules and other ingredients of the polymer material (pigments, stabilizers, reinforcing elements) in the course of processing. Novel processing methods need to be developed in the case of speciality polymers adapted to the requirements of their application in micro/macroelectronics, as medical implants or in portable energy sources (batteries, fuel cells).

(c) Transport properties

Polymers find important application in separation processes as active or passive membranes, adsorbents or chromatographic materials. In batteries or fuel cells they serve as ionconductors and separator materials. Much need exists to improve the relevant properties by understanding how the transport and dynamic phenomena relate to the molecular and supramolecular structures to be achieved by synthesis and processing.

1.6.5. Future Perspectives of Basic Research in Organic Materials Synthesis

(a) Synthesis by rational design

Progress in the computer-based simulation of expected behaviour of polymers in their respective application would greatly speed up the process of research and development in industry. However, the theoretical understanding of molecular interactions in the context of applications is in its infancy. Relevant software does either not exist or is unable to serve the purpose adequately. The same is true for the theoretical and computational handling of catalytic processes.

Better data on reaction kinetics and transport phenomena would greatly speed up and improve the production of polymers and enhance their performance as speciality or enabling materials.

Reactive extrusion or – more generally – reactive processing is another topic where rational approaches supported by computational methods would have an enormous impact.

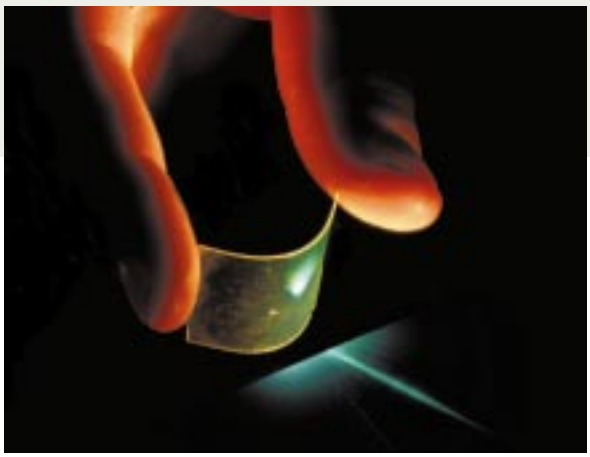

Fig. 1.11. A flexible coated polymer foil is able to transfer white light into blue/green laser light.

(b) Structure-properties correlations

Further development of analytical methods to characterize the structure and performance of polymers in space and time domain are prerequisite to further improve these materials. Fast *in situ* techniques of determining the molar mass distribution in the polymerization and/or processing step have high priority. Similarly, analytical techniques to allow for precise determination of the primary structure (branching, hyperbranching, crosslinking etc.) are presently too imprecise and awkward to have an impact in industry. Thus, novel high-speed analytical methods need to be found.

(c) High-purity synthesis and materials

Speciality polymers need to be adapted to the specific purpose of their application. This requires in many cases the development of new routes to synthesis and processing because of the required and necessary purity conditions. Examples are ubiquitous in biomedical applications (no toxic byproducts allowed) or in electronics (migration of even traces of byproducts will deteriorate a device).

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1.7. Carbon Materials

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1.7.1. The Chemical Complexity of Carbon

Elemental carbon in its chemical allotropes of graphite and diamond occurs in a great variety of species and has been developed to a large number of highly specialised applications as structural and functional materials. The underlying reason for this unique manifold of species is twofold:

- The co-ordination chemistry of carbon is flexible in allowing continuos mixtures of C=C and C-C bonding in one structure. This leads to an infinite possibility of 3-dimensional structures and to continuous tunability of electronic properties from wide-gap semiconductor (diamond) to metallic (graphite).

- Carbon accepts foreign elements such as hydrogen, boron, oxygen, and nitrogen both on its surfaces and within the structural framework. This leads to tunable mechanical properties from superhard (diamond, C-B-N) to ultrasoft (lubricating graphene layers). The surface functional groups determine the self-organization (aggregation in dyestuffs, laser toners), the chemical stability (oxidative attack in structural applications), and the reactivity towards stoichiometric (adsorbent) and catalytic processes (synthesis of small molecules, gas mask filters).

This complexity was augmented in recent years by the creation of mesoscopic composites on the basis of carbon-reinforced carbon materials (CFC). The manufacture of such materials for structural applications in the aerospace industry involves careful control of all points mentioned above and is an example of a super-complex material synthesis.

Carbon plays a major role in nano-sciences. Fullerenes, nanotubes, whiskers, carbon onions are typical representatives of nano-structured carbons to which all the above mentioned variables also apply in addition to the small scale of each object.

1.7.2. Current Applications of Carbon

Diamond as CVC diamond, as diamond-like carbon (DLC) and as homo-epitactic diamond plays a strategic role in electronics industry (protective layers on chips and hard disks, high power transistors) and in the cutting tool industry (blades for metals and silicon cutting).

Large objects of graphitic carbon are used in metallurgy (electrodes for furnaces), as heat shields (in space crafts, high temperature ultra-clean furnaces, fusion reactor machines) and as functional parts in motors (pistons in Otto motors).

Carbon fibres are large-scale products used as reinforcement structures in polymers and metals. Electronic applications as cables, heaters and supercapacitors are under development or existing in niche applications.

Carbon composites are widely used as electrodes in batteries (Li-ion types) and in electrochemical analytics. These applications draw on the ability to intercalate foreign atoms in the structure of graphite reversibly for batteries and on the ability to completely suppress this process by producing helically wound ribbons of graphite called “glassy carbon” for their apparent inertness and mechanical stability.

1.7.3. Future Application Potentials

All areas of application still require intense research and technological development as in none of the areas mentioned above where carbon is unrivalled by other materials, there are specific and limiting shortcomings of the materials properties.

In recent years a long list of other promising applications was produced by proponents of the novel forms of carbon. In all these potential areas of interest carbon is, however, competing with other material solutions under development. Almost all of these application potentials are, in addition, extremely speculative and may materialise only in the far future. A quite incomplete list of such potential application is given here:

- Nanotubes as electrodes for flat panel displays
- Nanotubes as hydrogen storage device (probably already falsified)
- Nanotubes for quantum wires

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- Nanocarbons in quantum electronics
- Endohedral fullerenes as "second periodic table" modifying the properties of all elements known
- Endohedral fullerenes as diagnostic drug
- Fullerenes in polymers
- Fullerenes as non-linear optical materials
- Fullerenes as anti-cancer drug

In such application areas carbon materials are only a system component. Neither the system development nor the basic science for the application is in a stage yet as to give specific instructions to carbon material scientists for a targeted evolution as possible with the applications mentioned in Sect. 1.7.2. In this area basic science with a wide scope for property discovery is required before any serious assessment of potentials and risks can be made.

1.7.4. The Scientific Community

Carbon science is an active field, interdisciplinary between physical chemistry, inorganic and organometallic chemistry and solid state physics. In the last 35 years the field has seen five waves of fashionable developments which have left wide areas of unknown material science and variations on the themes of wide gaps of fundamental understanding of carbon properties. These waves of fashion were:

- Carbon as nuclear materials (high-temperature reactor and graphite-moderated reactors)
- Graphite intercalation compounds as synthetic metals
- CVD diamond and superhard materials
- Fullerenes
- Nanotubes

The waves of activities have fragmented the communities substantially as the available funding is fluctuating drastically as a consequence of high promises and little technological successes in the short timescales of 3-5 years typical for funding campaigns. The application mentioned above required decades of continuous efforts to mature to the present standard. Despite large conference series the respective communities rarely find and work together with the consequence of a strong lack of coherence and frequent re-inventions of known facts.

In Europe, France, and Spain are the strongest national carbon communities followed by British and German groups who are particularly strong in application-near material science. Worldwide, the Japanese community is by far the largest and most active group followed by the European groups and by the North Americans. The Japanese and Spanish communities are growing and re-juvenating whereas most other communities are stable or shrinking. The fluctuation in active groups is very large with a tendency of the core competence groups to move out of the area for lack of long-term funding.

1.7.5. Research Bottleneck and a Breakthrough Opportunity

The extremely flexible chemical and hence physical properties of elemental carbon allow for a extreme variability in applications. Thus, in nanoscience as well as in conventional materials science the present applications are by no means exhausting the potential of the element. In order to exploit this potential it is urgently necessary to better understand the underlying chemical and partly physical properties.

The single most important problem for all applications is as mentioned above the rudimentary understanding of formation principles and restructuring processes of carbon. The generation of carbon is today a highly empirical and not very efficient procedure if specialized carbons are considered. The bulk carbons like carbon black for tyre industry or coke for metallurgical applications may be an exception to this but even there massive improvements in the production processes (superior application properties, sustainable production by lower energy input) seem to be possible as consequence of a better atomistic understanding of the thermal processes. In all high-tech applications the achievement of the desired properties is so expensive in labour, materials, and, in particular, in energy that large-scale applications such as in car industry (for structural applications) or in chemistry (for catalysis) are cost-prohibited. Without a driver of large-scale application it is difficult to expect that any industry alone takes on the research efforts required. Public funding is scarcely available as there is little interest in carbon science at present after all the disappointments with the promises from the waves of fashion.

1.7.6. Chances for an European Action

Europe could take the international lead in carbon materials science with a programme aiming at a science-based synthesis strategy for functional carbons. The German-Swiss-Austrian research initiative in CVD diamond manufacture and superhard materials was an impressive forerunner to such a project. A centre of excellence in Karlsruhe on CFC materials and strong groups in diagnostics,

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modelling and analysis of adventitious carbon in flames and automotive devices (soot formation) are further ingredients to such a network together with the traditional carbon groups. Essential work packages would be:

- Theory of carbon formation
- Elementary processes of carbon formation (graphite and diamond)
- Mesoscale physics and chemistry of primary carbon particles (aggregation of basic structural units, diamond micro-crystals , nanocarbons etc.)
- Surface science of carbon (adsorption, restructuring, surface defects and reactivity)
- Surface and aqueous chemistry of carbon (functional groups, aggregation processes, oxidation, reduction)
- Evaluation of the C-H-O phase diagram, search for novel phases and structures
- Defect chemistry and dynamics in carbon Mechanisms of high temperature processes and annealing (graphitization, chemical erosion)
- Novel precursor chemistry (polymers, mesophase)

Fragmentary knowledge does exist in all these areas. No coherent and experimentally sound picture has been achieved so far. Much unknown facts are bridged, however, by qualitative concepts with little experimental underpinning (see, e.g., the erroneous expectations on hydrogen storage in nanotubes which were put forward without knowing the adsorption data of hydrogen on graphite as a fundamental quantity for estimating maximum adsorption capacities). The replacement of these qualitative concepts by quantitative models removing the traditional separation between diamond and graphite science which is outdated since the discovery of materials with a variable content of sp^2 and sp^3 carbon groups should be a major goal of the network. It would be essential to bridge the gaps between the communities of graphite science, diamond materials science and nanocarbon science. If these groups could work together and adopt their respective paradigms to the knowledge already available, a substantial step forward in rational synthesis and planful modification of material properties of carbon can be foreseen. The network should not aim at the generation of specific products but rather build a technology platform enabling industry for the implementation of improvements. A wider materials basis would stimulate many areas of application and could remove the myth about a “high-tech” material of carbon which hinders its widespread application according to its wide span of properties. Such a programme would finally allow to better assess the long-term system potential of nanocarbon in larger areas of technology.

1.8. Electronic and Photonic Materials

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1.8.1. Introduction

Nowadays, it is well established that the possession and control of *information*, in its proper sense defined as news or knowledge, is regarded to have similar importance as crude materials like oil. To gain the desired information in time often decides about the commercial progress of an industrial company and, more general, of the national economy, respectively.

The introduction of the personal computer, and probably most important, the generation of the worldwide operating Internet has driven the transition of the civil community to the so-called “information society”: any kind of information is always open for everybody if it is made available via Internet in the World Wide Web. Thus, since the beginning of the 90's, the number of Internet users increased exponentially making the Internet to an important economic factor (keyword: e-commerce).

The various fields of the Information Technology in our understanding include the processing and transmission of information, as well as their display and memory. Those fields undergo a strong modification since their introduction. An overview about the corresponding research and development areas is presented in Fig. 1.12.

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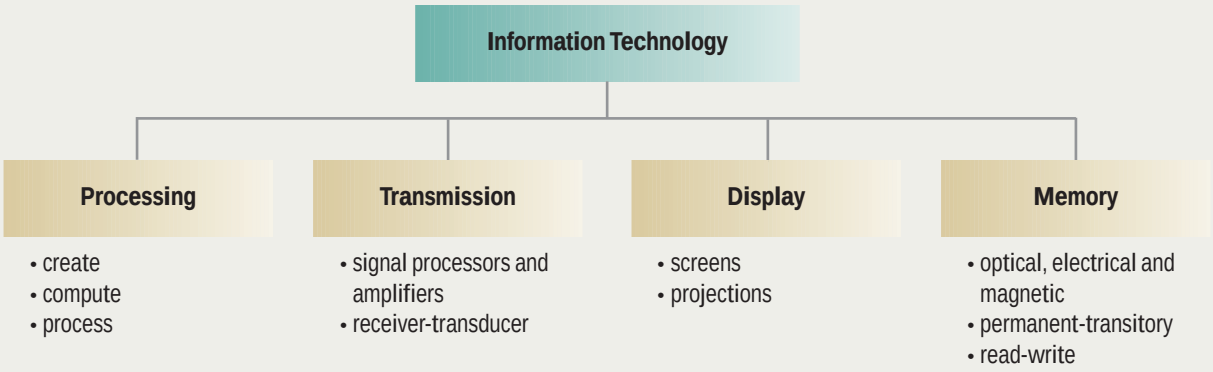

Fig. 1.12. Overview of the various fields of the Information Technology and their present research areas.

The credo of modern Information Technology seems to be very simple: making everything smaller, faster, cheaper - issues which are strongly interrelated and thus reaching into the broad spectrum of electrical, chemical, communication and computer industry. In the past two decades, these issues were one of the most important driving forces for the enormous economic growth within these industrial fields. This should be pointed up by means of the following current example: Since the announcement of high-brightness GaN-based blue light emitting diodes (LEDs) by Nichia Corporation in 1993, a worldwide market for these devices has developed. After six years, the market has already grown from zero to more than $400 millions in 1999. With the introduction of the blue-violet laser diodes based on nitride materials, the development of next-generation optical storage systems (e.g. DVD drives) is just running. The market forecast for both GaN-based optoelectronic and electronic devices is shown in Fig. 1.13. The total device market is projected to grow over $4.5 billion within the next 8 years!

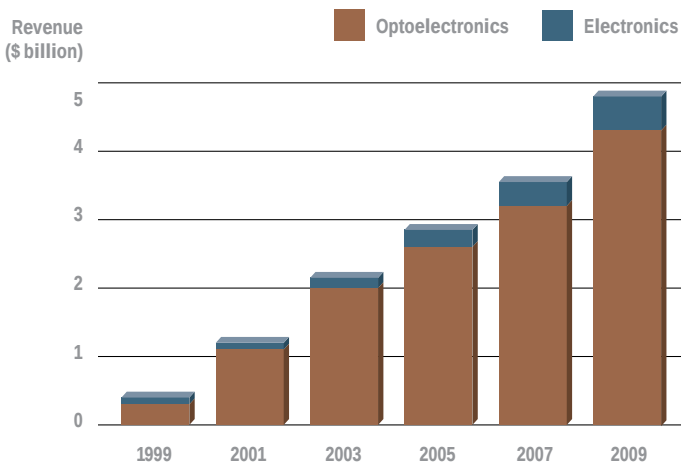

Fig. 1.13. Market forecast for GaN-based optoelectronic and electronic devices [1].

1.8.2. Present Situation – State of the Art

Since the early 70's, device fabrication in the microelectronics industry, the leading branch of Information Technology industry, has followed Moore's law in describing an exponential behavior for the reduction of the characteristic length scales of the devices (Fig. 1.14). This reduction in the size of circuit features, going ahead with higher number of operating units per chip, simultaneously results in an exponential increase of processing power and thus in higher device performances. This fact is the main reason for the formidable financial success of the microelectronic industry.

If following Moore's law for the next decade, the minimum device size will approach the 100 nm-range and the minimum gate oxide thickness will shrink to a few nanometres, respectively (Fig. 1.14). However, as feature sizes in electronic circuits move into the nanometre-size regime, fundamental physical limitations begin to emerge that are indicated by the transition from classical to quantum physics. These limitations include rather obvious issues, such as the non-deterministic behaviour of a small amount of switching charges, as well as basic quantum mechanics issues, like size quantization opening up significant gaps between energy levels and the ease of electron tunnelling through ultra-thin insulating barriers. Furthermore, the technological limits have to be overcome. For instance, a standard lithographic technology is not yet available for structuring down to nanometre-scale sizes; and, the fundamental problem has to be solved that future nano-devices should have lower power consumption.

The Semiconductor Industry Association (SIA) has developed a roadmap [2] enforcing limitations of the conventional scaling approach. This roadmap defines the continued improvements in miniaturization, speed, and power

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reduction in the information processing devices: sensors for signal creation, logic devices for operating, storage devices for memory, displays for the visualization, and transmission devices for communication. As a concrete example, the specifications for electronic devices after the year 2010 are summarized as follows:

- Feature sizes in the order of 30 nm or smaller
- Over 10^8 transistors per cm^2 for logic
- Over 10^{10} bits per cm^2 for memory
- A cost of less than 50 µcent per transistor for logic
- A cost of less than 600 ncent per bit for memory
- Operate at greater than 10 GHz
- 1.4 billion devices must consume less than 170 W

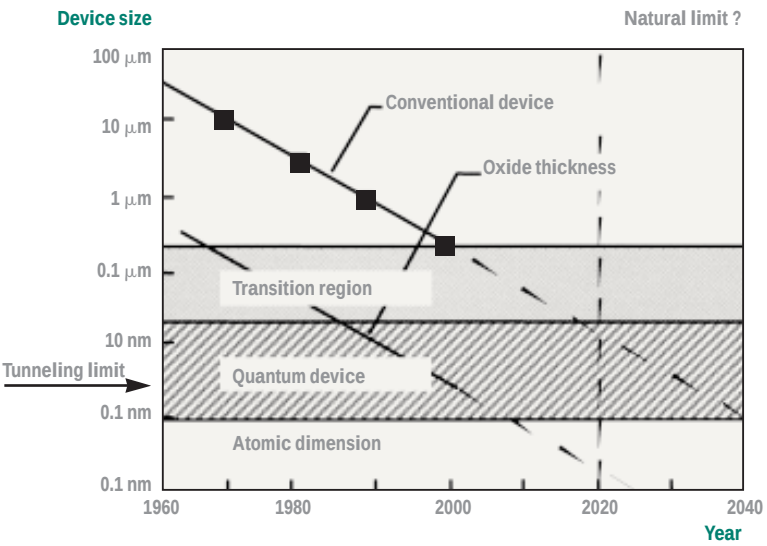

Fig. 1.14. Device size and oxide thickness vs. time scale demonstrating Moore's law. Critical limitations and novel research fields are indicated.

Such mandatory demands can only be realized with dramatic changes in fabrication technologies, device principles, and circuit architecture that has to include the development of *novel materials and material combinations*. The time for science maturing into industrial technology is approximately 10 - 15 years, this means that the time for starting these new research topics is just now.

Nanotechnology, and in particular nanoelectronics, is regarded worldwide as the key technology for the new century [3]. Strong advances in nanofabrication already allows the realization of electronic, optical, and magnetic artificial structures in atomic dimensions operating on the basis of quantum phenomena. The giant magneto-resistance effect, the quantum cascade laser or the single electron transistor should serve as only three prominent examples. In this context, the question about suitable and tailored materials will become more and more important because materials properties can be changed with the reduction of their dimensions and the portion of surfaces and interfaces will strongly increase compared to the volume. Thus, the interface itself will be dominant and will even control the function of the low-dimensional heterostructure. Semiconductors like silicon and silicon carbide or the III-V compounds including the group-III nitrides, respectively, will remain the basic materials, but the syntheses of new components and the combination of very dissimilar materials under well-defined conditions with novel functionalities will become more important.

Diverse statements are emerging in these days and discussed with respect to their potential to solve the problems appearing with the above mentioned demands. Besides, two possible ways are distinguished, the evolution of conventional information processing and the revolution of information processing, following different visions.

1.8.3. Evolution of Conventional Information Processing

This rather traditional route is based on the continuity of the conventional technologies such as the well-established "top-down" miniaturization approach combined with thin film technology. In the top-down approach, smaller structures are created from larger ones with lithographic techniques. However, this way has to include a miniaturization procedure adjusted with new lithographic methods and materials systems in order to reach the nm-range.

Although, the most important basic material will be silicon, because of its low price, mature sophisticated technology and compatibility to other existing technologies, the development of new materials and combinations with silicon will be inevitable. Fig. 1.15 presents an overview about the potential research areas for application of new functional electronic and photonic materials arranged in various fields of Information Technology. In the following, some of the most important material problems are summarized.

(a) Materials for lighting

The illumination market for incandescent and fluorescent light bulbs amounts to more than $1.5x10^{10}$ US$ per year worldwide with increasing tendency. The introduction of white light emitting diodes (LEDs) offers the advantage of increased lifetime and of economized energy. Thus, replacing all conventional bulbs by white LEDs would result in a saving of energy equivalent to the production of 38 nuclear power plants. However, to be successful, the internal

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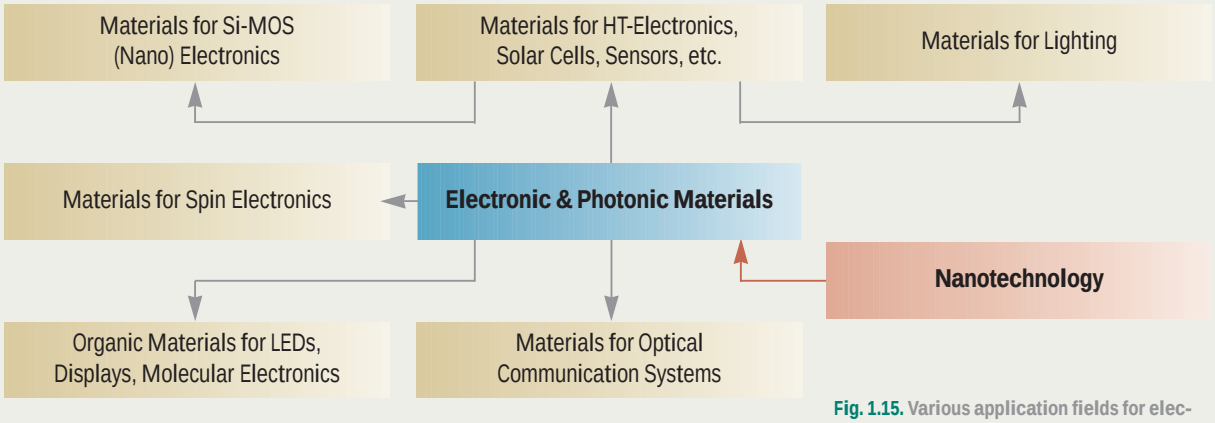

Fig. 1.15. Various application fields for electronic and photonic materials and the input of nanotechnology.

quantum efficiency of the LEDs has to be improved. For this purpose, basic materials problems have to be solved, primarily, the development of UV/Blue/Green LEDs and, linked with it, to find best qualified substrate materials for their heteroepitaxy, i.e., for the oriented growth of thin layers with high structural quality and perfect interfaces.

(b) Materials for Si-MOS electronics

The market of Si-based semiconductors is still larger than $1.5x10^{11}$ US$ per year. Materials research and development in this well-established field is mainly focused on constituent materials that comply with the scaling law in order to reach 10^{1} bits/cm^2. However, at the same time, the power consumption should be less than 150 W for 10^9 devices on one chip (cf. SIA roadmap).

One of the emphasized problems in Si-MOS electronics is based on the development of high-K materials, for example, replacing the amorphous SiO_2 as gate insulators. The optional material must naturally be compatible to the Si-technology and should, therefore, combine the properties of high thermal and chemical stability with a perfect wetting behaviour to the Si surfaces. Potential candidates are listed in Table 1.3 that additionally includes current issues and problems.

Option	Issues/Problems
Si_3N_4/nitride	small advantage, especially with buffer layer close to being ready
Ta_2O_5	need SiO_2 buffer / no poly-crystalline gate very early stages
TiO_2	need SiO_2 buffer / no poly-crystalline gate very early stages
(Ba, Sr)TiO_3	deep states / buffer layer / no poly-crystalline gate early stages FET (large DRAM interest)

Table 1.3. Gate materials for Si-MOS electronics with issues and problems.

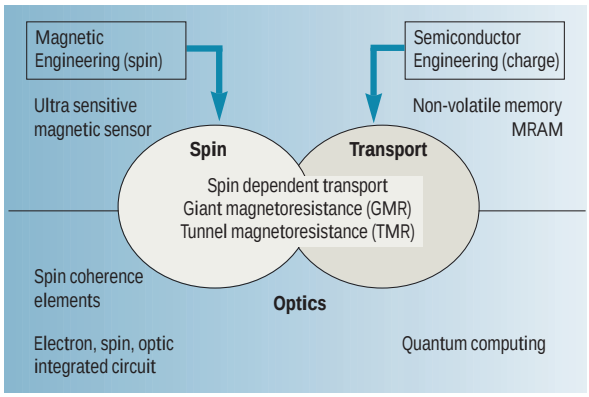

Fig. 1.16. General concept for spin-electronics, after ref. [5].

(c) Spinelectronics

The concept of spin-electronics is summarized in Fig. 1.16, where the combinations of magnetic and semiconducting technologies are displayed. Both, the spin and the charge of electrons contribute to new functional devices and will probably break the limitation of existing device concepts. Specific material aspects are still at the beginning, as it is reflected by the introduction of many diverse material combinations and concepts for the realization of magnet-semiconductor hybrid structures (e.g., ref. [4]).

In general, the large potential of spintronics can conveniently be recognized by the giant magneto-resistance (GMR) effect that only needed 10 years from discovery to implementation in commercial devices. Further feasible applications are given in the figure.

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(d) Materials for optical communication systems

Beside the high operating frequency of the electronic integrated circuits, the band width, i.e., the amount of information transmittable over a single fibre strand, is a key factor for the total transfer rate that can optimally be reached. This band width double every 9 to 12 month that is twice the innovation of Si-MOS technology, consequently requiring an enormous spectrum of technical innovations (see overview in Fig. 1.17).

New materials for laser diodes and novel concepts for laser fabrication are necessary in order to be able to extend the wave length range. For instance, the artificial and thermodynamically unstable quaternary (In,Ga)(As,N)-system is investigated as basic material for the generation of lasers emitting at 1.5 µm wavelength [6].

The idea of novel all-optical devices, i.e. switches, modulators, filters and interconnects, seems to be possible with so-called photonic-bandgap materials: materials patterned with a periodicity in the dielectric constant, which generates a range of "forbidden" frequencies, called *photonic bandgap*. Photons with energies within this bandgap cannot propagate through the material. This will allow to control and manipulate the propagation of light even within compact systems of very small dimensions.

Nevertheless, essential material-related questions generally remain concerning the improvement of the process control, the stability and purity of the soft films and composites, non-ideal metal/organic contact, and about the reduction of the power consumption. For example, if we take into consideration that the energy difference between highest and lowest occupied molecular orbital is typically 1 eV and that the contact resistance is assumed to be about 100 Ω, the power consumption of a single electronic device would then be 0.01W. Realizing an integrated circuit with 10^{10} devices (typically for CMOS device) would result in 10^{8} W (i.e., a nuclear power station to run it!). This result is independent of the circuit architecture used. Most of the experimental measured resistances are in the range of MΩ to GΩ, therefore, a substantial improvement or different thinking in Integrated Circuit-architecture is required.

(f) Nanotechnology

An alternative process is the use of nanostructures for electronic applications. Nanoelectronic devices might be implemented in a circuitry by "bottom-up" approaches while maintaining the conventional circuit architecture (Boolean algebra). In general, the bottom-up approach is realized as follows: small structural blocks are built from atoms, molecules, or from single device level upward. The method principally allows the precise positioning of the building blocks and hence their functionality. The essentially

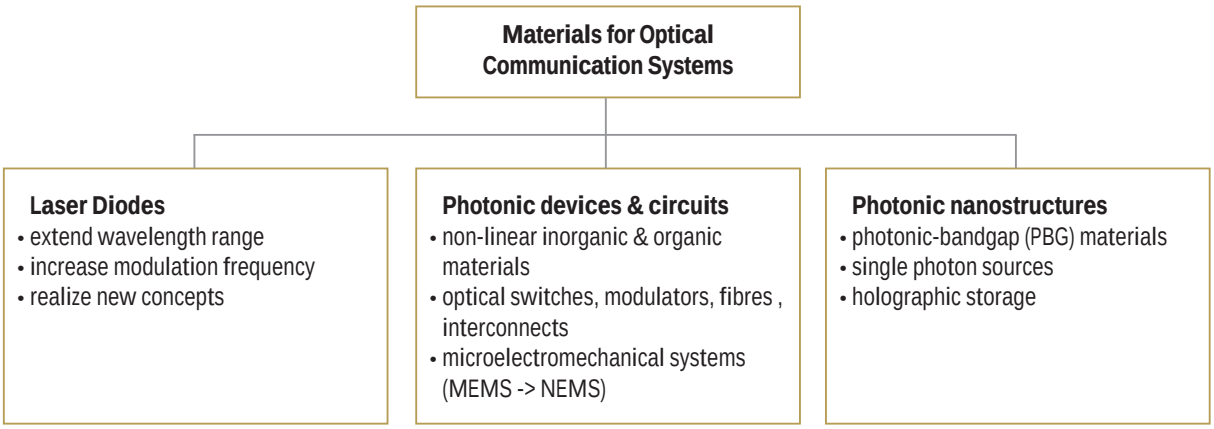

Fig. 1.17. Overview of research areas for materials for optical communication systems.

(e) Organic materials for LEDs, displays, electronics, etc.

The vision of unlimited engineering flexibility through direct control of molecular orbitals combined with low-cost fabrication techniques has been made organic materials very attractive. Organic light emitting devices for large area projectors or the imprint technology for "paper-like displays" are going to be successful in commercial fabrication [7].

high integration level is achieved with self-assembled or self-organized functions – the most critical key issues for a successful transfer to industrial products (like for instance in single electron transistors). Proposed solid state device implementation at this level has therefore to solve the following essential problems:

(1) controlling the critical dimension (tunnel barrier height or the quantum dot size),

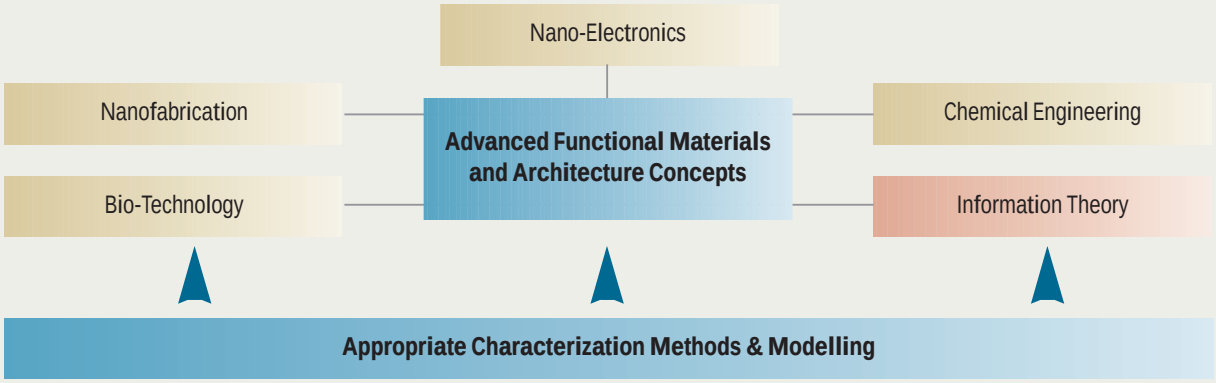

Fig. 1.18. Combination of innovative research areas as the driving force for developing new materials in the Information Technology

(2) the reduced operating temperature, and
(3) the interconnection and the alignment of the nanostructures.

Ultimately, a conceivable scenario to avoid the problems (1) and (2) is to build ultra-dense and low-power nanoelectronic circuits made from purely nanometre-scale switches and wires. Specific individual molecules are able to act as wires and switching devices ("molecular electronics") combining the primary advantage that these molecules are natural nanometre-scale structures which can be produced absolutely identical and in vast quantities by synthetic organic chemistry. The electronic properties are, however, still almost unknown. Again, the problem of heat dissipation is still unsolved as already mentioned in the previous section about (e). Materials understanding and materials processing are thus basically necessary for a further successful development of this molecular electronics.

Alternatively, bio-molecules are introduced in nanoscale devices: DNA templates act as programmable scaffolding upon which the electronic components can precisely self-assembled. The transfer of information along the DNA seems to be possible without the problem of significant electrical resistance (intra-molecular electronics), but many issues are unsolved.

(g) Nano-fabrication and characterization

Prerequisite for nanoelectronics is the development of nanoscale measurement tools, standards, and fabrication methods. Tools for visualization and characterization are vital for understanding nanoscience in its variety and for understanding the nature of nano-manufacturing processes, too. Those smart nanoprobe techniques have to be accurately sensitive to electronic, magnetic, structural, chemical or biological properties as well as the specific combined functionalities. The techniques of microscopy and nanoanalysis based upon electrons, ions, photons and scanning probes are key assets.

Nanoprobe techniques for manufacturing prototypes (atom-by-atom manipulation in the STM) are already used on a laboratory level containing single nano-device structures for investigating and testing their functionality.

1.8.4. Revolution of information processing

This route is more innovative and revolutionary because it does not rely on conventional research principles. In addition, it assumes pro-active strategies with long-term visions for the knowledge-driven innovative materials research.

In the Information Technology arena, nanodevices will both enable and require fundamentally new information processing architectures that are radically different to present existing. Feasible examples are quantum computing, or to DNA like data processing systems. This approach implies that the information processing principles based on general information theory should be more inspired by natural biological than artificial physical systems (non-Boolean algebra). However, before being able to integrate those basic systems in a novel information technology, they have first to be understood in more detail, i.e., their physical, chemical, and biological structures and processes.

In a second step, advanced materials and, in particular, heterosystems based on materials with very dissimilar properties are then necessary in order to combine biologic and microelectronic information processing principles ("bio-electronics"). Here, a new kind of materials engineering for interface creation and manipulation must be

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developed as well as novel concepts in the packaging technology (e.g., for the device resistance against outside).

While device and circuit concepts are highly speculative in this area, the combination of innovative ideas from nanotechnology, nanoelectronics, biotechnology, and information theory together with appropriate characterization tools and theoretical modelling will offer promising ways for realizing revolutionary technologies in the future. This kind of advanced materials research is therefore a strongly interdisciplinary field, as illustrated in Fig. 1.18.

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1.9. Nanotechnology and Semiconducting Materials

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This contribution is centred on two strongly connected fields. We first discuss the major trends in nanotechnology and stress its importance in a wide variety of applications. We then examine what can be a possible evolution in basic research on semiconducting materials.

1.9.1. Some Aspects of Nanotechnology

(a) Introduction

One of the main motivations for working at the nanoscale comes from the evolution of microelectronics towards miniaturization. This is contained in the famous empirical Moore's law which states that the number of transistors per chip doubles every 18 months (Fig. 1.19)

Such an exponential increase serves as a guideline for the roadmap of silicon-based microelectronics. The ultimate goal is to reach 10^{11} bits/cm^2 instead of the 10^7-10^8 realized at the present time. However this reduction in size induces new effects, e.g., errors due to charge offsets, quantum confinement effects, etc., which already manifest themselves in the smallest laboratory transistors with a gate length of 20-30 nm. At the industrial level the normal attitude is to follow the roadmap and try to solve the technical problems associated with each generation of devices. There is consensus that this trend must end up in 2012 with a minimum feature size of 35 nm.

It is thus necessary to prepare new solutions if one wants to pursue this trend further. One approach is to start from the ultimate limit, i.e. the atomic level, and design new materials and components which will replace the MOS based technology. This is exactly the essence of nanotechnology, i.e. the ability to work at the molecular level, atom by atom, to create larger structures with fundamentally new molecular organization. This should lead to novel materials with improved physical, chemical, and biological properties and, in turn, to exploit theses properties in new devices. Such a goal would have been thought out of reach 15 years ago but the advent of new tools and new fabrication methods have boosted the field.

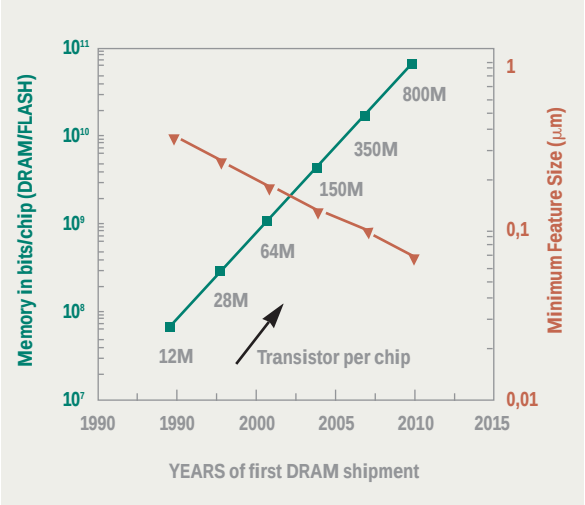

Fig. 1.19. An example of Moore's law.

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(b) Some elements for the future

We only consider some aspects of the tremendous development expected in the field of nanotechnology.

Our central point will be nanoelectronics. As discussed before the estimated end of the roadmap is in about ten years where problems relate both to the cost of fabrication and to the reduction in dimensions will occur. There are various ways to increase the integration. One of them is to perform 3D integration. There are already start-up companies in the U.S. working on such projects. In the future one might consider that self organization techniques could achieve this successfully. Of course there will be problems related to power dissipation and to connections in such systems. The last problem will also occur for 2D arrays of nanostructures and numerous studies concerning the realization of conducting wires have already started and should be intensified. Simultaneously, studies concerning new devices will be pursued. It seems to us that silicon will still remain the central material at the nanometre scale. Much effort should be spent on the realization of silicon based nanodevices. The physics of innovative device concepts and new approaches to nanostructures synthesis are essential to such development. Improved predictive simulation techniques and characterization methods will also be of central importance to the design of such new devices. This means that exploratory research is necessary on subjects like quantum size effects, tunnelling, exchange coupling, conductivity of nanowires, magnetic and ferroelectric properties at the nanoscale. Due to these new physical effects, the existence of quantum fluctuations and the importance of point defects new fault tolerant architectures will be needed and must be an active field of research in the near future. The operation at room temperature and the possibility of low cost integration into working systems are basic constraints for the applicability of such new devices.

Another rapidly emerging field is molecular electronics. The most classical aspect concerns light emitting diodes for flat panel displays, already at the industrial stage. One should note the first realizations of organic transistors with comparable performance to amorphous silicon. This allows the hope of an “all organic” solution to flat panel displays. Another source of application already in development is “plastic transistors”. However, the field which is closest to nanotechnology is electronics at the scale of the molecule. Here the ultimate goal is again 3D integration with 10^{16} bit/cm^3 i.e. 10^{13} logic gates/cm^2. There are already many studies but no clear cut demonstrations of electronic devices based on a single molecule yet. Among the numerous problems to be solved the following:

- Realization of molecular devices: diode, conductivity of a molecular wire, wiring and connections to electrodes.
- Self organization for 3D integration.
- Molecular circuit architecture (again fault tolerant).
- Connections and thermal dissipation.
- Use of DNA for the resolution of some algorithmic problems.

To the same field of research belong the rapidly expanding studies concerning the single-wall nanotubes (Fig. 1.20), the fullerenes, and other aromatic molecules which can give rise to molecular crystals with various optimized physical properties like superconductivity. This will certainly lead to new developments.

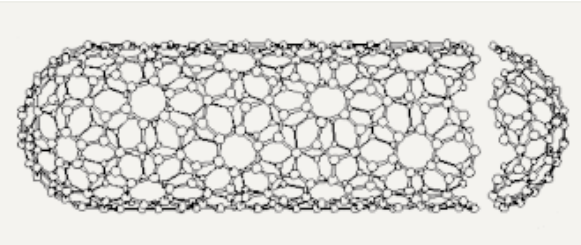

Fig. 1.20. Single-wall carbon nanotube.

To end up this list we must mention opto-nanoelectronics with the optical study of individual quantum dots and their use in optoelectronic devices. Another trend is the fabrication of photonic bandgap superlattices to guide and switch optical signals with nearly 100% transmission, in very compact architecture. With this in mind a remaining challenge is opto-electronic silicon. There have been hopes and disappointments concerning the possibilities of realizing silicon-based lasers. However, quite recently, optical gain in silicon nanocrystals has been demonstrated. The field of magnetic nanostructures is also rapidly expanding particularly due to the realization of devices exhibiting giant magnetoresistance. There is still basic physics to be done as well as improvements in magnetic storage. A similar situation is also emerging for ferroelectric memories (Feram's) where fabrication, characterization, and optimization studies are required. Another interesting problem is the behaviour of nanosized grains of ferroelectric materials.

Beyond applications to electronics and computing nanotechnology will, no doubt, lead to revolutions in the following: improved properties of materials for a variety of uses, medicine and health with new drug delivery systems for instance, environment and energy with integrated sensors allowing corrective action, biotechnology and agriculture, etc.

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As a final point in this list let us mention the parallel progress made in the context of micromechanical (MEMS) and micro-optomechanical (MOEMS) systems which have benefitted from the techniques of fabrication of microelectronics. These have for instance allowed the realization at the microscale of actuators, motors, mirrors, laboratories on a chip, etc. In view of what happens in living world (molecular motors) one can also expect reduction of size in this area. Together with progress in nanoelectronics, nanocomputing, integrated nanosensors this could lead to the advent of what might be called nanorobotics with enormous applications especially in health care.

(c) Conclusion

As mentioned in several papers nanotechnology is likely to be one of the leading fields of research and development in the next century. It will have a variety of applications in practically all domains. It must involve different disciplines like electronics, physics, chemistry, biology, etc. It should lead to the opening of new possibilities like quantum computing, optical computers, nanorobotics, with impact in nearly all economic fields.

1.9.2. Semiconducting Materials

The increasing importance of semiconductors is due to the fact that they have been and still are the basic materials for the technological revolutions of electronics over the last forty years. Electronics represents the most important market at the present time and the one that benefits from the fastest growth. It covers a wide range of industrial fields: computers, telecommunication, automobile, various mass products, military and space applications, etc.

In this global market, the part of semiconductors is in the order of 10 %. The basic material is silicon, the relative part of compound semiconductors increasing steadily.

(a) General considerations

The dominant field of application is microelectronics (mostly based on silicon) but others like audio and microwaves as well as optoelectronics are increasing at a rapid pace. Technologies inherited from microelectronics have also allowed the emergence of new fields: microsystems and micromechanics coupling sensors, micromotors, actuators, and microelectronics. As discussed before an essential feature of microelectronics is the tendency towards increased integration which obeys Moore's law.

The expansion of semiconductors is not limited to that unique aspect. In the past audio and microwave applications have been stimulated by military needs. Now the interest has shifted to commercial mass markets: cellular phones, size reduction of devices, improvement in transmission quality and efficiency, increase in power and distance, etc. In these fields compound materials are increasingly important (e.g. GaAs, InP, GaN, SiC). In optoelectronics the compound semiconductors are used to obtain laser diodes for nonlinear optics. They play an essential role for fast modulation of light. In all cases, one also has a tendency towards decreasing size with growing importance of quantum phenomena.

The limits of the field are not clear cut. First of all progress is not confined to applications but can also allow important discoveries in basic physics, like the quantum Hall effect. On the other hand devices of the future will be increasingly based on coupling between semiconductors and other types of materials: normal or superconducting metals, magnetic materials, various dielectrics, molecules, biological systems, etc. Control of the corresponding interfaces is essential. This implies interdisciplinarity involving cooperation between chemists, biologists and specialists in microelectronics and computer science.

(b) Subfields

We list here a number of key subfields (areas of long term research are marked by the sign*)

i) Silicon based integrated circuits Elaboration and characterization of very thin dielectrics (< 5 nm) for gate control – new types of dielectrics – very thin junctions (< 10 nm) – interconnects (electromigration) – reliability of few electron memories and difficulties related to quantum fluctuations * – strain induced problems – growth, plasma or chemical etching of films – progress in lithographic techniques – the possibility of optical interconnects * – optoelectronic silicon *.

ii) Large gap materials These materials have a major interest for optoelectronics. Some of them like Zn Se, diamond, SiC despite an indirect gap, the nitrides GaN, InN, AlN allow to cover a broad spectral band. Another field of application is microelectronics in hostile environment and power electronics. The difficulties to overcome are typical for materials studies: growth techniques appropriate to a reduction of native defects – choice of substrate – control of dopants – use in microwave and optoelectronic devices. Heterostructures and superlattices: These systems lead to applications in microwaves, optics (in particular nonlinear optics) and to optoelectronics. The focus will be on a better control of the layers, in particular for strained layers where the creation of dislocations must be avoided (for instance via metamorphic growth). III - V compounds,

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of strategic importance, are among the best candidates to reach ultimate performances in microwaves. On the other hand it is necessary to pursue studies on Si Ge in order to improve the already remarkable results obtained with this compound. With regards to optics, further work is needed on optical microcavities, semiconducting or dielectric Bragg reflectors as well as photonic band gap materials.

iii) Nanoelectronics and nanophysics This represents long term research on the elaboration and characterization of basic materials for tomorrow's electronics. It is essential to pursue studies on the following subjects (non exhaustive list): – single electron devices memories, transistors * – lithography at the nanometric scale: X-rays, electrons, STM – near field spectroscopies applied to the characterization and fabrication of nanosystems * – deposition of self-organized layers on semiconductors: grafted molecular layers, elaboration of wires, quantum dots and superlattices of 3D crystallites: eventually application to optoelectronic silicon * – coupling of semiconductors with organic molecules with a given functionality or with biological molecules * – interfaces between semiconductors and dielectrics, superconductors or magnetic materials ; application to new devices (e.g spin transistors)* – mechanical switch or memory of atomic or molecular size * – use of the remarkable properties of fullerenes, nanotubes and other forms of carbon * – development of new appropriate (fault tolerant) circuit architectures* – quantum computing *.

iv) Non electronic micro- and nano-devices This is a rapidly expanding field with micro-electro-mechanical systems (MEMS) or even micro-opto-electromechanical systems (MOEMS) (pressure sensors, accelerometers, micromotors), microfluidic devices (e.g. micropumps, microvalves), chemical or biochemical sensors as well as optical microdevices. These realizations have benefited from the technologies derived from microelectronics. Here again, aspects related to thin layers of semiconductors are essential. The future lies in the design and realization of new types of devices, of so called smart systems, in the search of specific applications. In a more distant future one can foresee an evolution towards a reduction in dimensions, eventually down to the nanometric scale*. The association with nanoelectronic systems might lead to micro and nanorobotics *.

v) Unconventional semiconductors Some new semiconducting materials synthesized in chemical laboratories might present extremely interesting properties. This was the case for instance of skutteridites for thermoelectricity. Another example is provided by tin or antimony chalcogenides which are potentially useful for microbatteries as well as infrared optoelectronics. In all cases coupled physico-chemical studies are needed in order to optimize the materials with respect to the desired properties. Another aspect concerns semiconducting polymers which have recently exhibited potentialities for electroluminescence and the realization of so called plastic transistors.

vi) Theory and simulation The field of microelectronic devices has benefitted for some time from the use of simulation and modelling techniques. These are mostly based on the resolution of macroscopic equations incorporating a simplified representation of the material in terms of parameters (effective mass, diffusion coefficients, etc.) which are often fitted to experiment. Progress in computing techniques will make these approaches more and more realistic, microscopic processes (e.g., diffusion barriers) and electronic states being better described. Numerical codes will be incorporated in the description of the behaviour of real devices. Efforts will be needed to describe the different steps in the realization of devices: growth, implantation, and lithography.

Finally the reduction in size towards nanometric scales together with the ever increasing computational power begin to allow direct application of ab-initio quantum calculations to realistic systems. Much work obviously remains to be done in this field which must lead to the possibility of engineering *a priori* the physical properties of elementary components.

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Conclusions

In this chapter the need for basic research for the different categories of materials has been discussed. The categories cover metals and metallic alloys, ceramics and other non-metallic, inorganic materials, polymers, organic materials, carbon materials, and electronic materials. Even within the traditional categories of materials there is plenty of research to be done into new and poorly understood phenomena. In particular, connections need to be made between the chemistry, microstructure, and properties of materials in all classes.

A detailed analysis of the different groups reveals that there are four important areas of research common to each: (1) the science of processing, (2) the science of characterisation, (3) measurement of properties and (4) theoretical modelling of properties based on the microstructure. These four aspects have to be dealt with on different length scales. Fundamental aspects of materials based on quantum chemistry and physics needs to be connected to microstructural units and large-scale structures by multi-scale approaches. Until recently, processing of materials was performed predominantly on a mesoscale level (in the micrometre range), but growing interest in nanomaterials means that we will soon be able to design materials from the atomic and molecular levels.

The tasks awaiting us in the future are manifold. On one hand it is important to continue to improve existing materials (such as steels) by controlling the microstructure and/or composition (microalloying). On the other hand, research into novel materials still has great potential simply because of the large number of elements in the periodic table. So far only two- and three-component systems have been systematically investigated to any significant degree. New compounds and materials with extraordinary structural or functional properties can be discovered by experimenting with a wider range of elements and additives. These studies should be guided by well-grounded theory and computer simulation to make the most efficient use of time and resources. However, it is difficult to predict the behaviour of materials with complex microstructures, so further breakthroughs in the area of modelling (see Chapter 4) are needed.

Nanotechnology is an important topic for all classes of materials. One aspect of nanotechnology is the processing of materials composed of nanoparticles (nanopowders) where net-shaped materials can be formed. However, this is only possible if grain growth can be avoided or drastically reduced both during processing and when in use. The other aspect of nanotechnology is to build new nano-sized components. These components are important where speed is a critical factor for, e.g., nanoswitches, nanoelectronics. Experiments have been performed to determine the properties of materials consisting of small numbers of atoms or arrays of atoms, e.g., nanowires. An enormous amount of work still needs to be done, however, before nanotechnology can achieve its potential.

For the EU to generate and benefit from new breakthroughs in materials science, room needs to be made for fundamental, “blue skies” research in all categories of materials. The many sources of inspiration, imagination, and innovation in the European science community need to be supported by such forward-thinking policies if Europe is to remain one step ahead of other regions investing heavily in materials research.

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2. Materials: Science and Application

Introduction

In this chapter materials are discussed in terms of specific applications for different technologies. One of the most important and challenging areas for man-made materials is in biology and medicine. Biomaterials can be thought of as covering two separate but related areas: replacement of human organs and body parts, and "biomimetics", where we seek to synthesize materials by imitating processes and structures found in nature.

Biomaterials currently used in human implants were not developed specifically for this purpose, but have been selected from pre-existing materials. This has meant that interactions between the implant material and natural tissue have not yet been thoroughly examined. Ways of improving this situation are described in several sections of this chapter.

In biomimetics there are different approaches to understanding the function of structural hierarchies in biological systems. Both the "bottom-up" approach and the "top-down" approach can provide interesting insights into Nature's way of producing lightweight, tough materials in the most efficient manner.

The science of catalysis is also a very important area described in this chapter. So far knowledge of catalysis (heterogeneous as well as homogeneous catalysis) has been gained mostly by empirical methods. Unfortunately, there are barriers to the flow of information in catalysis research due to the substantial economic interests involved.

Optical and optoelectronic materials are of increasing importance since optical communication is widely regarded as the future of information technology. The materials being developed range from amorphous materials (glasses) to semiconducting and organic compounds. The magnetic and superconducting properties of various materials are used in a number of essential applications, and this work was strongly supported under the 5th Framework Programme. A great challenge will be developing materials for use in nuclear fusion reactors. This includes structural materials for the reactor superstructure as well as plasma wall materials stable at extremely high temperatures.

Materials used in the transport industry are developed by a number of different research communities. The main aim is to create lighter, stronger and cheaper materials for use in mass transportation systems (ships, aircraft, cars, trains). Reliability is a critical issue.

The study of materials in Space is another new field that may generate a better understanding of processing and microstructure than could otherwise be achieved by doing the same experiments on Earth. Interesting results can be expected.

Successfully developing materials for specific applications requires close interaction between scientists and engineers both in academia and industry. Many of the examples described in this chapter show that Europe has the imagination, ability and experience to achieve this.

◀ Domain structure in ferroelectric $BaTiO_3$ (transmission optical micrograph obtained with polarized illumination, U.Täffner, MPI für Metallforschung Stuttgart).

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2.1. Biomaterials: Evolution

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2.1.1. Introduction

There is a big demand for biomaterials to assist or replace organ functions and to improve patients' quality of life. Materials options include metals, ceramics and polymers. Unfortunately, conventional materials are used that were not specifically developed for biological applications. Interaction between biomaterials and natural tissues is an important subject for biomaterial science (see Fig. 2.1). Such information is essential to aid the design of new biocompatible biomaterials.

2.1.2. State of the Art [Metallic, Ceramic and Polymeric Biomaterials]

Biomaterials are widely used in medical and dental treatments but their effectiveness is questionable. Almost all were developed for general use. Some alloys and hydroxyapatites were introduced in orthopaedic and dental fields and satisfactory results were obtained. Hydroxyapatite has the advantage that it connects to natural hydroxyapatite in bone (see Fig. 2.1). Toxicity must be avoided but inertness is not a high priority in biomaterials. Unfortunately, metallic and ceramic biomaterials are not suitable to replace soft tissues because of markedly different mechanical properties. Conventional polymers are used for many of today's disposable medical devices but new functional biomaterials are awaited.

2.1.3. Future Visions: Evolutionary and Revolutionary; Breakthroughs

Replacing natural organs with artificial ones causes difficulties when they do not function properly. However, artificial organs are necessary to support part or all of their essential functions thereby improving quality of life. Artificial kidneys are one example. At present artificial hearts are only used temporarily to keep patient alive prior to organ transplantation. Availability of transplantable organs is strictly limited. New functional biomaterials are needed to improve artificial organs.

Non-thrombogenic artificial surfaces are an essential target for synthesis. There have been many proposals to provide blood-compatible surfaces. Immobilization of heparin and urokinase, and introduction of poly(ethylene oxide) chains on the surface are promising but they do not have generality. Accumulation of plasma proteins on the blood-contacting surfaces must be minimized. Preparation of multi-functional biomaterials, such as non-thrombogenic elastomers and permeable membranes, is a future challenge.

2.1.4. Future Research Needs & Priorities

Artificial organs must be connected to our bodies during use but methods of connection still need to be researched (see Fig. 2.1). Infection at the interface is an unsolved problem in medical devices and artificial organs. Encapsulation around implanted biomaterials is a remaining problem, which is essential for implantable bio-sensors. Other problems in artificial organs are how to join each artificial blood vessel with the patient's natural vessels. It is not yet possible to get durable bonds between artificial organs and human tissue. Biocompatible blood access is also required for dialysis patients.

Good scaffold is needed for cells and tissues other than gelatine and collagen. A three-dimensional bio-matrix is important for tissue engineering, especially to make hybridized artificial organs such as artificial liver support system.

2.1.5. Highlighting Internal Research Programme Needs

Hard dental tissues do not have effective wound-healing characteristics and do not regenerate; this was not initially realized by dental researchers and clinicians. Clinicians believe they could provide durable prostheses to fix defects but the cut tissue did not heal and suffered invasion by micro-organisms. This is termed 'secondary caries'. More importantly, even today, it is not possible to connect artificial materials to natural tissues (including tooth substrates). It has been argued that adhesive technology should provide the option of better dental treatments.

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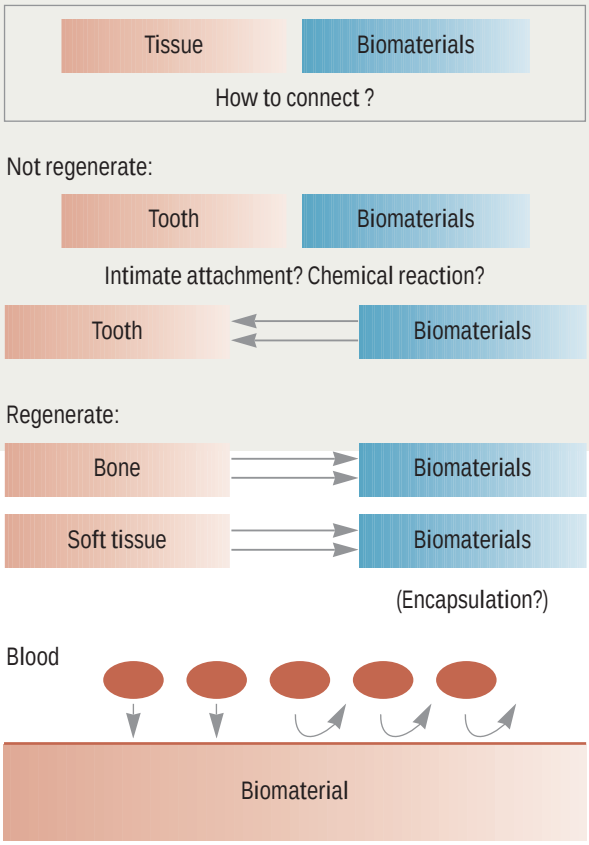

Fig. 2.1. Interaction between biomaterials and natural tissue.

Initially, loss of tissue needs to be minimized during the treatment. Nakabayashi has developed new technologies which give tooth substrates pseudo-wound-healing characteristics; these could revolutionize dental treatments (-see Fig. 2.1). Hybridized dentine and enamel are created on the subsurface of tissues by impregnation of monomer resins, followed by *in situ* polymerization. It is expected that hybridized dental tissue, together with impermeable and acid resistant artificial enamel, could resolve many current problems in dentistry. Education in dental schools must be changed to introduce this new technology widely into dentistry. Dental biomaterials may then eliminate many defects in dental hard tissue and rejuvenate their function.

Non-thrombogenic biomaterials are widely used in the development of artificial hearts but there are difficulties in their preparation. Artificial hearts are available as a temporary measure to bridge the transfer during heart transplantation even without non-thrombogenic substrates. The inner surface of blood vessels is composed of 'biomembranes' whose main components are phospholipids. It has been suggested that methacrylate with phospholipid polar groups might be used at the membrane interface as the polymer surfaces could accumulate phospholipids when in contact with body fluids. 2-Methacryloyloxyethyl phosphorylcholine (MPC) has been prepared and the characteristics of copolymers were evaluated. Such copolymers are non-thrombogenic, highly hydrophilic, permeable, translucent and do not accumulate bio-active proteins on the surface. Bio-compatibility of several artificial surfaces could be improved by coating. There are now several promising multifunctional biomaterials available, which are being applied to new types of artificial organs and advanced medical devices. This technology could open up revolutionary new fields in biomaterials research. MPC and the copolymers are commercially available from NOF Co., Yebisu, Tokyo 150-6019, Japan.

2.1.6. Conclusion – Recommendation

Patients with several handicaps require new type biomaterials to improve their quality of life by assisting, recovering and/or reconstructing diseased or lost functions/organs. Lack of good bio-compatible biomaterials requires development of tissue engineering. For example dialysis membranes keep more than 500 thousand chronic kidney patients alive every year. Tissue engineering has limitations and work is in hand to prepare new functional biomaterials, with sufficiently strong mechanical properties. MPC polymers are an example. Good scaffolds are also needed for tissue engineering. Biotechnology, based on gene science offers useful, if difficult methods of producing effective materials for medical devices and artificial organs.

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2.2. Biomaterials: Research and Development

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2.2.1. Introduction

Biomaterials are either modified natural or synthetic materials, which find application in a wide spectrum of medical and dental implant and prosthesis for repair, augmentation or replacement of natural tissues. Some well-known examples of the clinical use of biomaterials are total joint replacement, vascular grafts and heart valves. However, such implanted prostheses are still generally based on materials selected from engineering practice (designated as *first generation* biomaterials), which combine the ability to be tolerated by the body with mechanical properties sufficient to withstand anticipated physiological stress. While providing an effective immediate solution for many patients, the outcome is often time-limited. As a consequence, there has been considerable research interest in investigating mechanisms contributing to implant-prosthesis failure and in the potential for developing second generation biomaterials with extended lifetime in the patient.

A key feature of *bioactive*, rather than biotolerant, second generation biomaterials is that the interfacial reaction between the implant and its surrounding tissue is controlled, with the normal cellular processes being encouraged. Hence, this approach to the design of second generation biomaterials for particular clinical applications is an example of *in situ* tissue engineering, which is an approach particularly suited to bone replacement. Considerable progress has also been made in tissue engineering external to the body; and, through cell multiplication and matrix expression in bioreactors, it has proved possible to develop analogues of tissues such as skin, cartilage and ligament. Such advances provide a basis for a progression towards the ultimate of organ replacement, with benefits in terms of quality of life for patients and in opportunities for associated industry.

Biomaterials as an international priority – The importance of biomaterials in the U.K. has been highlighted in three national reports. From an users end, a Department of Health report [1] identified orthopaedics, dentistry, urology, wound repair, ophthalmology, cardiology and vascular disease as "*clinical specialties where biomaterials play a significant role in healthcare delivery*." This report complemented an earlier report from the Institute of Materials Strategy Commission [2], which commented that "*biomaterials saves lives, relieves suffering and improves the quality of life for a large number of patients every year*." In addition, the Office of Science and Technology "Foresight" exercise [3] identified biomaterials as a priority topic within the materials sector and recommended "*substantial increased resources in...a new generation of biomaterials which encourage and enhance the restoration and repair of body tissue function*." In the U.S., it is well accepted that the three fields poised for explosive intellectual and commercial growth in the 21st century are molecular biology, information science and advanced materials [4]. Biomaterials bridges two of these fields and includes research and training components in both basic science and applied engineering aspects. In Europe, hundreds of thousands of patients receive joint replacements, vascular grafts, and heart valves, each year, with each one having a finite lifetime *in vivo*. With an ageing population, an improved technology base is essential.

2.2.2. Bone and Skeletal Implants

(a) First generation biomaterials for bone and joint replacement

The functional demands on skeleton – and hence on bone, the major skeletal tissue – are rigorous, with requirements to enable upright stance, allow locomotion through muscular action, and provide protection for internal organs. Many people enjoy a lifetime of appropriate skeletal function, but for many other bones and joints become damaged or diseased and require replacement. Arthritis of skeletal joints - particularly hip and knees - is a major health issue and produces pain and loss of mobility, affecting both young and elderly patients. Osteoporosis, a crippling disease affecting particularly a large number of women over the age of 50 (and a smaller number of men as well), frequently leads not only to disfigurement but to serious bone fractures, such as of the femoral head or acetabulum of the hip joint.

The seminal work of Professor Sir John Charnley, an orthopaedic surgeon, produced an artificial hip joint to replace an arthritic hip joint, which was introduced in 1961. Today, hip prostheses based on Charnley's approach still constitute a majority of the 40,000 operations (hip arthroplasties) per year in the UK, 250,000 per year in the U.S.,

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and more than 600,000 yearly world-wide. Similar numbers of knee arthroplasties are carried out yearly. The popularity of these procedures notwithstanding, the original hip operation was designed for a 65+ year-old patient, with the expectation of prosthesis lifetime of about 10 years. This expectation has been achieved [5], but the progressive increase in patient longevity since 1961 and the application to younger patients, for whom a shorter prosthesis lifetime is obtained (decreasing to rather less than 2 years for a 40 year-old patient [6]), have resulted in an increasing demand for repeat operations, or *revision surgeries*. By 1995, the percentage of revision hip procedures performed in the U.K. has increased year-by-year to 18% [1] and to a comparable fraction in the U.S. Materials selection for Charnley's original design was based on first-generation biomaterials, viz a stainless-steel femoral stem and polyethylene acetabular cup, both "cemented" (or, more accurately, grouted) in place with poly(methylmethacrylate) bone cement. Similar approaches have been taken for artificial knee joints, with a femoral condylar component of stainless steel or Co-Cr alloy articulating against a polyethylene tibial insert. Such materials, derived from current engineering practice in non-biological applications, have in general not themselves failed under physiological conditions.

However, what was not anticipated was the effect of joint prostheses on the biology of the surrounding bone, which is living tissue, maintained in an equilibrium state by the continuing activity of bone cells (osteoblasts making bone, osteoclasts resorbing bone). The combination of stress shielding of adjacent bone by a prosthesis stiffer than bone, sometimes exacerbated by the inflammatory cellular response to particulate wear debris, lead to bone loss with time and an eventual loosening of the prosthesis, 79% of hip joint failures actually arise from *aseptic* loosening. These two critical functions of mechanical matching and biological compatibility must therefore be addressed if the lifetime of the prosthesis is to be increased. Ideally, a once-only operation, with an extended prosthesis lifetime of 25 years or more, is required. Such an horizon for hip joint replacement extends to all systems used for bone repair and replacement in the skeleton – in the treatment of other joints such as the knee, in bone cancer, in fractures, and in congenital, traumatic or accumulated bone defects, such as those arising in osteoporosis and periodontal disease.

(b) Second generation biomaterials

The limitations of first generation biomaterials have stimulated research to develop optimized prostheses for joint replacement, utilizing biomaterials more closely resembling the biological template. A radical innovation was the introduction of synthetic hydroxyapatite, $Ca_{10}(PO_4)_6(OH)_2$, a calcium phosphate compound which approximates to the bone mineral phase that comprises about 45% by volume and 65% by weight of human cortical bone. It was demonstrated that, in the body, hydroxyapatite (HA) performed as a bioactive material and promoted bone apposition to the surface rather than encouraging bone resorption. The seemingly innate propensity for implants to loosen appeared to be reversed, a finding of considerable importance. The commercial availability of hydroxyapatite powders led to the introduction of a femoral stem coated with plasma-sprayed hydroxyapatite, to be used as a *cementless* system for a younger patient group, and spawned a whole industry of HA-coated dental implants. The suggestion is that enhanced early fixation into bone will improve prosthesis lifetime, even though the biomechanical mismatch of implant and tissue remains. There have been conflicting data as to the long-term efficacy of this approach, but a major clinical trial has recently demonstrated a positive outcome for a younger age group over a 12-year follow-up period [7]. An extensive post-mortem study of retrieved hip implants in elderly patients has also revealed that, in that population as well, HA maintains a more intimate integration of bone with implant [8].

Hydroxyapatite has also found clinical application as a generic bone graft material, and much attention is being given to the development of porous HA for tissue guiding, with the prospect of application as bone graft in revision joint fracture repair and spinal fusion procedures.

Currently, the materials demand is satisfied mainly by using real bone, either the patient's own living bone from other sites (autografts) or dead bone from cadaver or other sources (allografts). Use of a synthetic substitute obviates the pain and surgical complexity of autografts and the risk of infectious disease transmission from allografts. The requirements for the substitute appear deceptively simple, viz to supply a porous matrix with interconnecting porosity, which promotes rapid bone growth, yet possesses sufficient strength to prevent crushing under physiological loads during the interim bone growth process. A key recent development has been better understanding of the role of substituted ions in hydroxyapatite in the biological response. By making synthetic HA more closely resemble the chemistry of natural bone mineral, it has proven possible to speed the integration of implanted material into bone. Most promising is selective incorporation of carbonate [11] and silicon [12] ions, which may reduce osseointegration from 28 days to 7 days, a dramatic potential benefit for patient treatment.

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(c) Commercial innovation in bone biomaterials

A notable example of the innovation of a second generation biomaterial, is provided by hydroxyapatite-reinforced polyethylene composite (now designated HAPEX™) for use as a bone analogue pioneered by Bonfield *et al*. [9]. Modelled on the structure of cortical bone as a natural composite of collagen fibres and apatite, HAPEX™ was tailor-made to provide matching deformation characteristics and superior fracture toughness to cortical bone, so as to produce bone apposition rather than bone resorption at an implant surface. The concept was developed with incremental testing and processing to produce an optimized composite, which entered clinical trial as a suborbital floor implant [10]. It was established that HAPEX™ could be trimmed readily by the surgeon to fit precisely the skeletal defect and promoted bone bonding without the need for cement.

In 1995, HAPEX™ was licensed by a British company, Smith & Nephew plc, and manufactured by its ENT Division in the U.S. for application as a trimmable shaft in a middle ear implant (replacing the partially or totally damaged or diseased bones which transmit sound from the diaphragm to the inner ear). Following approval by the Food and Drug Administration, HAPEX™ was launched at the American Academy of Otolaryngology in late 1995 and achieved immediate clinical take-up with its advantages of trimmability, providing a precise fit to the individually varying middle ear space, and of bonding to the residual bony base. Clinical follow-up has indicated a very satisfactory restoration of hearing [11]. By 2000, HAPEX™ had been incorporated into 22 different designs of middle ear implant, with benefits already to about sixty thousand patients, as well as from wealth creation for the associated industry. HAPEX™ provides a salutary example of tailor-making a second-generation biomaterial for a particular medical implant, and demonstrates the progression from laboratory concept to commercial application in patients. From this base, other implants for bone replacement or augmentation became possible, with commercial potential for a range of minor and major load-bearing applications, including maxillofacial reconstruction, spinal prostheses and revision hip prostheses.

(d) Bone formation and osteoporosis

Bone is living tissue comprising bone cells (osteoprogenitor cells, osteoblasts, osteocytes, osteoclasts) and a blood supply, encased in a strong composite matrix defined by interwoven fibrous proteins (collagen, adhesion proteins). The matrix is distinguished from that of other connective tissue by being significantly (45% by volume, 65% by weight) mineralized and organized into lamellae. Osteoblasts cells, which derive from progenitor stromal stem cells, are responsible for formation and remodelling of bone matrix, in particular in rapidly developing bone such as that growing to appose implanted prostheses; osteocytes are osteoblasts which have become embedded in bone matrix. Osteoclasts, which arise by differentiation from hemopoietic stem cells, are responsible for resorption of bone, largely through local acidification, which dissolves bone mineral and permits a range of proteolytic enzymes to destroy the associated bone matrix. Living bone is continually undergoing remodelling from the opposing action of osteoblasts and osteoclasts.

Bone matrix is natural composite biomaterial with a complex hierarchical structure. It comprises bundles of collagen fibres which have been infiltrated by a crystalline mineral phase, resembling synthetic hydroxyapatite, $Ca_{10}(PO_4)_6(OH)_2$, but in which some of the tetrahedral $[PO_4]^{3-}$ phosphate groups have been replaced by planar $[CO_3]^{2-}$ carbonate group, F- or Cal- ions can substitute for some $[OH]^-$ groups, and the crystal structure more closely resembles that of the hexagonal fully fluorine-substituted fluorapatite. As the carbonate content is increased, HA crystallites gradually adopt a plate-like morphology. Electron microscopy studies by Professor Hobbs' group and others have shown that collagen and the apatite mineral form continuous, independent, interpenetrating networks.

Cortical bone is the dense bone (~10% internal porosity) making up the shafts of long bones like the femur (thigh) or tibia (shin). *Cancellous* – or *trabecular* – bone has an interconnecting porous architecture (50-90% porosity) made up of curvilinear struts called *trabeculae*; it appears at the ends of long bones – where hip and knee implants are fixed – and in the vertebral body. In the process of new bone formation, for example adjacent to femoral stems in hip implants, osteoblasts migrate to the wound site, attach, and within days release collagen which forms an immediate fibrous template for mineralization to form new bone matrix. The rate and direction of bone matrix formation and resorption is influenced by stress in the bone arising from loads imposed by gravity and muscle action, which is why bone atrophies in idle limbs or in space.

Osteoporosis is a disease state in which resorption of bone matrix takes place at a faster rate than creation of new bone matrix, so that the normal remodelling balance is upset, leading to a decrease in bone density and strength. The World Health Organization has defined the diagnostic criterion for osteoporosis to be bone with a bone mineral density of more that 2.5 standard deviations below the young adult level. The two most common types of fractures associated with osteoporosis are those of the hip (proximal femur) and spine (vertebrae). Each year in the United States

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there are 250,000 age-related hip fractures, with an estimated health care cost approaching $10 billion and 700,000 age-related vertebral fractures, with costs of £1 billion. In Britain, the equivalent overall costs approach £2 billion. Hip fractures in the elderly are associated with excess mortality rates of 12-20% above that which would normally be expected. Almost all hip fractures are associated with trauma, such as a fall, while most vertebral fractures are the result of the activities of daily living.

Whereas in the proximal femur the cortical bone carries a high proportion of mechanical load, particularly in the mid-neck and shaft, in the vertebrae, most of the load is carried by trabecular (cancellous) bone. Between the ages of 30 and 80 years, bone mass generally decreases by 1%/year; in patients with osteoporosis, trabecular bone loss can decrease by up to 9%/year. On average, women lose about half of their trabecular bone over their lifetime, corresponding to a 75% reduction in strength. Clearly, changes in the mechanical properties of osteoporotic trabecular bone increase the risk of fracture.

2.2.3. Prospects for Tissue Engineering

Bioactive composites for bone substitutes, such as HAPEX™ provide an approach to skeletal regeneration in which the implant surface provides a favourable site for the recruitment of cells from the surrounding biological environment, with the subsequent cellular processes leading to the expression of matrix and tissue formation. In cellular or tissue engineering, such cells are cultured outside the body to form tissue that can be used subsequently for tissue repair. The primary advantage of a tissue substitute obtained by this route is that some or all of the biological growth factors would be immediately available, rather than needing to be recruited. Such an approach has particular appeal, for example, in the potential repair of regions of healthy cartilage damaged by injury, as a more conservative treatment than that of total joint replacement. There are enormous intrinsic challenges in the production *ex vivo* in a bioreactor of tissue comparable (in terms of composition and properties) to normal natural tissue.

Other key challenges are to develop a source of cartilage cells (chondrocytes) with a favourable immune response, to design an appropriate method of fixation, and to provide effective storage. With respect to cartilage, companies such as Advanced Tissue Sciences in the U.S. have taken the pioneering work of Langer [12] through to prototype cartilage grafts, which approach (but do not yet equal) the composition and properties of the natural tissue. One exciting prospect is of conditioning the cartilage cells in culture in the bioreactor by mechanical stimulation, so as to produce an equivalent or even superior tissue. When available, a competent cartilage graft will have enormous implications for the early treatment of defects in articular cartilage, both to repair damage in healthy tissue and in the first stages of arthritis.

For other tissues, such as skin, both *in vivo* and *ex vivo* approaches have been developed. The seminal work of Yannas [13] on the biomechanics of skin provided the basis for his development of a porous polymer-based scaffold to recruit fibroblasts *in vivo* for skin regeneration. Alternatively, tissue-engineered skin from a bioreactor is now in clinical use for the treatment of diabetic foot ulcers.

For bone tissue engineering, there is a direct link from the research on porous hydroxyapatite, which could provide a suitable matrix delivery system for osteoblasts or precursor stem cells. In the former case, such an approach would provide an autograft equivalent to bone grafting, without the need for a second operation. An exciting prospect in the latter case is the production of both bone *and* cartilage through cell differentiation locally directed by scaffolds and scaffold chemistries, so as to produce a mini-implant of cartilage already in place on bone, e.g. a replacement acetabulum of bone complete with its cartilage lining, which would eliminate the considerable difficulty of fixing cartilage to bone *in vivo*. A complementary approach is to stimulate osteoblast recruitment, e.g. by local delivery of parathyroid receptor agonists through prior transfection of the PTH gene into local fibroblasts.

2.2.4. General Conclusions

First generation biomaterials have made possible the existing procedures for bone and joint replacement now in current use, which provide restored mobility and relief from suffering for many thousands of patients on a worldwide basis. However, the advent of novel second generation biomaterials and the prospects for tissue engineering offer the potential for a broader range of longer lasting implants and prostheses, with benefit both to patients in terms of quality of life and to the associated industry in wealth creation.

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2.2.5. Research Priorities for Europe

- More European programmes of a scale to compete with major developments in the U.S. and Japan (and potentially China).
- At the same time, develop collaborative programmes with key centres in the U.S. (following the Cambridge University-MIT model).
- Develop a distinctive materials science approach to embrace the continuum from gene to protein to cell to biomaterial to medical device.
- Emphasize the innovation of novel biomaterials and tissue-engineered artefacts, based on the biological template, for tissue and organ replacement.
- Develop an understanding of the mechanisms controlling the interaction of cells with second-generation biomaterials and third generation tissue engineering scaffolds.
- Encourage the progression of novel biomaterials from the laboratory to distinctive clinical applications in patients by entrepreneurial technology transfer.

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2.3. Biomaterials: Medical Viewpoint

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2.3.1. Introduction

The field of biomaterials – materials working under biological constraints – is rapidly expanding. It is considered that this domain represents 2 to 3 percent of the overall health expenses in developed countries. For example France spends every year 30 to 40 billions of French francs. World expenses could be estimated at 100 billions of dollars.

This field covers a lot of different materials: cardiac artificial valves, artificial vessels, cardiac stimulators, stents, artificial hips, knees, shoulders, elbows, materials for internal fracture fixation, scoliosis treatment, materials for urinary tract reconstruction, artificial crystalline, skin, ears ossicules, dental roots and so on. Many different materials are involved: *metals* i.e. titanium alloy, cobalt chromium alloy, stainless steel, tantalum, *ceramics* i.e. alumina, zirconia, hydroxyapatite, calcium carbonate, *plastics* i.e. polyethylene, polymetylmetacrylate, polyurethane and also *composites*: carbon-carbon, natural materials i.e. coral, nacre, bovine collagen and so on.

Some new fields are now explored such as cell therapy or growth factors therapy that need some supporting material which is a very expending field.

2.3.2. State of the Art on Biomaterials Research

It is an interdisciplinary field. Many different experts must work together. Mechanical engineers, material scientists, chemists, biologists, medical doctors, and surgeons have to meet in interdisciplinary teams dedicated to this subject. They must also keep in touch with their originated field in order to be aware of up-to-date research in their specific domain.

This interdisciplinary field of applied research is very linked to industry. Industry is very aware of quick development and income, governments and administration are aware of controlling expenses, prices and security. Academic research is not developed, neither in Europe nor in

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the U.S. Interdisciplinary work could result in a serious breakthrough not only for insuring security and comparison between different materials but also to understand several basic problems that are totally uncontrolled. For example, the way living tissue react to foreign materials, what are the law of reject or acceptance, how living cells react to mechanical changes in their environment, how could it be possible to enhance tissue regeneration, tissue fixation on artificial surfaces, how to develop materials that will not break under mechanical stresses. Many problems are already solved but as a new field, few institutes or national sciences foundation are aware of that. Since this is not a recognized discipline, there are very few structured teams, few facilities, limited amount of public money, no position available if no discipline exists and so on.

This could be one of the major issues at an European level to promote this field of research in different scientific communities like mechanical engineers, physicists, chemists, biologists.

2.3.3. Future Expected Breakthroughs

An effort might be made in developing overlapping and links between the different scientific communities that might be needed to develop projects. Subjects are numerous from simulation methods, mechanical as well as numerical, new adapted materials, phenomenological research on cells, tissues, organs behaviour when in contact or replaced by some artificial materials, functionalized materials that acquire a special biological affinity to answer a special question: anticoagulant materials on plastic surface, antimicrobial agent, anticancer drugs and so on. Exact mechanisms of cells linkage to artificial surfaces could have a major implication in material acceptance. At the time of cell therapy, there must be some teams implicated in tissue engineering who will work on stem cells that could be cultivated and then growth on different artificial supports to replace a damaged tissue: bone, skin, ligament, cardiac wall and so on. At the time of new products like growth factors are supposed to provide enhanced healing factors, materials for their delivery in selected tissues is also of major relevance.

Countries must also organise the results appraisal at a government level: quality control, patient register that allows to follow every implanted material and to know exactly the outcome of these implanted devices. This permits also to insure security and to quickly remote a product when failures are identified.

2.3.4. Guidelines, Orientation and Priorities of Future European Research

An EC action might take many directions. One could be to foster and promote this scientific field and develop basic research in academic institution. Public grants for basic research in conjunction with some mixed public and industrial funds on more applied fields might be promoted. Selected fields of interest might be considered like cells and artificial surfaces, mechanical modelling of living cells, quality controls of biomaterials including their behaviour after human implantation, ceramic dedicated to living materials replacement.
These actions at a European level could permit to identify interdisciplinary teams dedicated to the field and give them the possibility to work on a long term basis. Any limited action as it was done in the past were not strong enough nor prolonged and then after an initial enthusiasm, the teams just broke down.

In Europe there is an old tradition of excellent basic research in different fields that could be involved: engineering, chemistry, biology, materials science. Many researches were already developed in weapons, transports, and nuclear industry. The biomaterials field represents a field with very important consequences for the population. Any biomaterial that fails could be the reasons for death, disability, further surgical operation and this might convince our politics that this field might really be supported as a strategic one.

2.3.5. U.S., Japan, EU Positions

Rules are quite different for different countries. In the U.S., the Food and Drug Administration is very strict about new materials to be applied in human.

In Europe, these materials must have a EU mark that is given by some institutions that have been labelled by each government to deliver this mark. Then the product can be sold in every EU country and remains under the law of each country. For example in France, a law called “Huriet Law” describes the process of human experiments that has to be accepted by a technical committee before this material can be sold. In Japan, the field is quite developed because some cultural specificity forbids the use of human material or organ transplant. This explains why some materials like ceramics or cells supporting material are quite in advance.

Anyway, the market is actually dominated by the U.S. Even if their products are not the best, their implications in re-

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search and the strength of the industry is a way to promote their products, even if not totally up-to-date. For example many advances are originated in UK, Germany, France, Switzerland but finally developed and marketed in the U.S.

It is also true that the major pharmaceutical companies from Europe like Aventis, Bayer, Sanofi, Synthelabo and others are not involved or no more involved in this field for many historical reasons.

2.3.6. Conclusions

Biomaterials is one of the growing field in health care system in the world. Europe is no longer on the road for different reasons explaining why our exchange balance is negative. A massive input to foster and promote basic academic researches in the field could modify the scope. Europe has all the expertise to do so. Only political will is missing. Selecting this field as strategic and acting accordingly could be the answer. In order to organize this field, a bunch of experts might be nominated representing different medical areas like cardiovascular surgery, orthopaedics, ENT, ophthalmology, materials science. These interdisciplinary teams might work together in order to propose common actions, to nominate experts to select the best proposal and also to organize some centres of excellence in some of these fields that could handle some of these missions such as: evaluation, development, quality controls, basic research and link with the industry. One centre by area of interest and by major countries could be a bunch mark to start this effort. Also courses dedicated to biomaterials and organized at a European level could be organized.

2.4. Biomimetic Materials and Transport Systems

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Summary

Biological cells have amazing materials properties, which are based on their macromolecular and supramolecular (or colloidal) building blocks. During the last decade, much progress has been made in order to identify these different components and their interactions. The next step will consist in the integration of these different components into higher-level systems. Some examples for such biomimetic systems are: supramolecular architectures containing membranes and polymers; polymer networks as models for the cytosceleton; biomimetic mineralization; transport via molecular motors; biomimetic recognition and signal transduction.

These research activities are interdisciplinary and involve the combined efforts of physicists, chemists, molecular cell biologists and bioengineers. The biomimetic model systems, which will arise from these efforts, have many potential applications in bioengineering, pharmacology and medicine.

There are various places in Europe, which already pursue related research on a local scale. What is still missing, however, is an initiative, which combines these efforts on the European scale. Such an initiative is necessary in order to compete with the science community in the U.S. where several "BioX"-centres are currently being set up.

2.4.1. Introduction: The Goals of Biomimetics

Biological cells are built up from macromolecules and supramolecular assemblies (or colloids) in water. Both the intracellular architectures and the interactions between cells are based on soft and flexible nanostructures, which are multifunctional and highly intelligent materials. In addition, cells are able to build up hard materials in the form of biominerals and to control their morphology on the nanometre scale.

All cells contain similar macromolecules but different types of cells can survive in very different environments. Indeed, cells can live in boiling water, in strong acids, at the low temperatures of the Antarctic, and under the enormous pressures of the deep sea. These different adaptations, which are based upon different supramolecular architectures, demonstrate the wide range of possible material properties of these architectures.

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Another intriguing aspect of biological cells is that they contain a large variety of very efficient transport systems. The latter systems are based on motor proteins or molecular motors, which transform chemical energy into mechanical work. These nanoengines are responsible for the transmembrane transport of ions and macromolecules, for the regulated adhesion and fusion of membranes, for the intracellular transport of vesicles and organelles, for cell division and cell locomotion.

Research on biomimetic materials and transport systems has four goals:

- *Understanding* the material and transport properties of biological cells and tissues. Since these latter systems are very complex, such an understanding can only arise if one focuses on certain aspects of these structures. Thus, one is led to the
- *Construction of model systems* to which one can apply the experimental and theoretical methods of physics and chemistry. The coevolution of experiment and theory is a necessary condition in order to transform vague ideas into useful knowledge.
- The knowledge obtained from the biomimetic model systems can then be used in order to develop *new types of designed materials* which are biocompatible and which have defined physical, chemical or biological characteristics.
- *Applications* of these biomimetic materials in bioengineering, pharmacology and medicine.

2.4.2. State of the Art

The structural organization within biological cells has many levels. As one goes "bottom-up", i.e., from small to large structures, the first three levels are: (1) the level of macromolecules (or copolymers) which have a backbone of monomers connected by covalent bonds; (2) the level of supramolecular assemblies of many similar molecules, the formation of which is governed by noncovalent forces such as the hydrophilic or hydrophobic interactions with water; (3) the level of complex architectures which contain different types of building blocks and/or different types of assemblies. These different levels will be discussed in the following subsections.

(a) Recent developments: macromolecules

The macromolecular components of the cell (proteins, nucleic acids, polysaccharides, lipids) are known for a long time. All of these macromolecules are copolymers, which are built up from a certain number of different monomers or building blocks. In addition, the three-dimensional conformation of these biopolymers is determined, to a large extent, by the water solubility or hydrophilicity of these building blocks. From the viewpoint of material science, one simple and useful property of biopolymers is that all members of the same molecular species have the same length. In contrast, synthetic polymers always exhibit some length distribution or polydispersity.

In the last decade, new synthetic methods have been developed which allow the construction of hybrid molecules consisting of biopolymers coupled to synthetic ones. In this way, one can design new biomimetic polymers, which combine the properties of both the natural and the synthetic component. In addition, new experimental procedures, so-called "single molecule methods", have been established by which one can determine the physical properties of single macromolecules.

On the one hand, one can label these molecules by a fluorescent probe and then track their motion both in solution and bound to a sheet-like membrane or rod-like filament. On the other hand, one can firmly anchor them at a solid surface and then probe individual macromolecules by various experimental methods. Using optical methods, for instance, one can directly observe the thermally excited transitions between two different conformations of RNA strands. One may also use the tip of an atomic force microscope in order to pull at a single copolymer, which is anchored to a solid surface. In this way, one can determine the functional relationship between the force and the linear extension of the molecule. These force-extension curves are rather reproducible and, thus, reflect the forces, which determine the three-dimensional conformation of the polymer.

Fig. 2.2. Cartoon of two molecular motors, in this case two kinesins, bound to a microtubule filament. The microtubule has a thickness of 25 nm. Each kinesin walks along the filament by making steps of 8 nm.

A third area where single molecule methods have led to much insight is the active movement of molecular motors along filaments. For some cytoskeletal motors (see Fig. 2.2) it has been possible to resolve single motor steps, which are of the order of 10 nanometres. In the cell, these motors are responsible for the directed transport of vesicles and organelles over tens of micrometres or even centimetres.

(b) Recent developments: supramolecular assemblies

If one looks into a typical animal or plant cell, one sees two types of supramolecular assemblies which determine the spatial organization of the cell over a wide range of length scales: (i) compartments bounded by sheet-like membranes and (ii) networks of rod-like filaments. These two types of structures are displayed in Fig. 2.3 and Fig. 2.4. Both structures are assembled on the molecular scale, i.e., on the scale of a few nanometres, but are able to organize much larger spatial regions up to tens of micrometres!

Biomembranes are highly flexible and, thus, can easily adapt their shape to external perturbations. In spite of this flexibility, they are rather robust and keep their structural integrity even under strong deformations. *This combination of stability and flexibility* is a consequence of their internal fluidity. This was first realized in the context of lipid bilayers, which are the simplest biomimetic membranes.

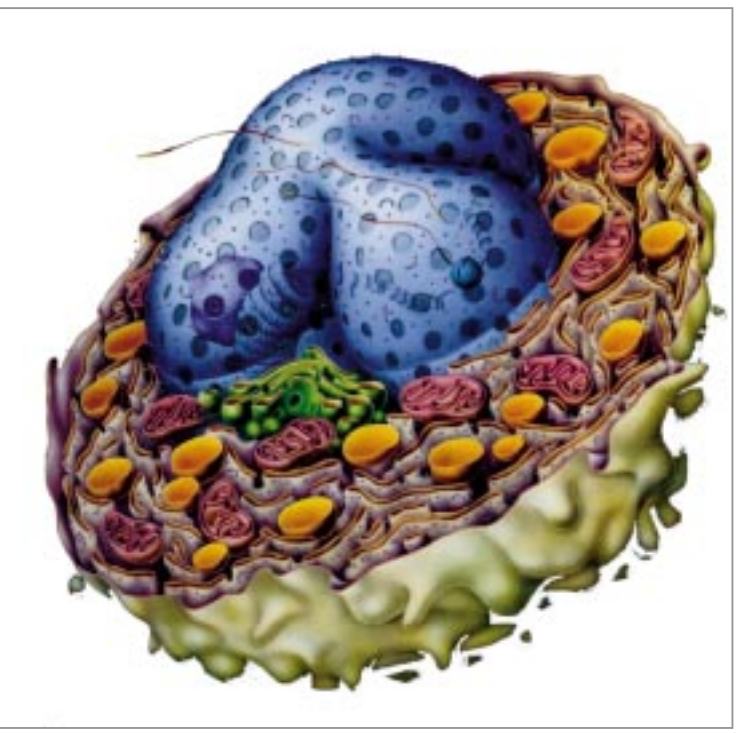

Fig. 2.3. The spatial organization of a typical animal cell is based on membrane-bounded compartments. The diameter of the cell is of the order of 20 micrometres.

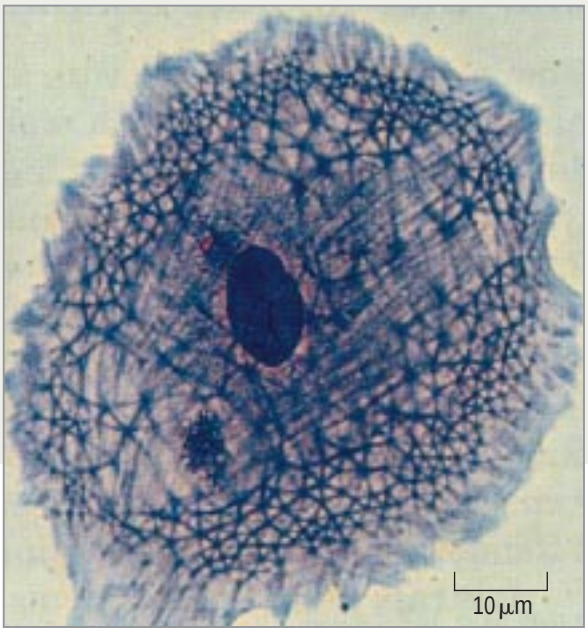

Fig. 2.4. Cytoskeleton of a large animal cell. This network of filaments is primarily built up from microtubuli, which emanate from the centre and actin filaments at the periphery of the cell.

Fluid membranes have unusual elastic properties, which determine their morphology. These properties are now understood in a quantitative way using (i) mesoscopic models which describe the membranes as elastic sheets and (ii) models with molecular resolution which can be studied by computer simulations and can be used to relate the elastic parameters with the molecular interactions.

The stability of lipid bilayers makes it possible to isolate them and to manipulate them in various ways: one can suck them into micropipettes, attach them to other surfaces, and grab them with optical tweezers generated by focused laser beams. These membranes are even self-healing: if one pinches small holes into them, the holes close again spontaneously.

In the last couple of years, new types of biomimetic membranes have been constructed. One example is provided by bilayers of amphiphilic diblock copolymers. Both artificial and hybrid copolymers have been found to undergo spontaneous bilayer formation. The underlying mechanism is the same as for lipids. Another type of biomimetic membrane is provided by polyelectrolyte multilayers. These multilayers are constructed in a layer-by-layer fashion where one alternatively adds negatively and positively charged polyelectrolytes onto solid templates. These multilayers form dense polymer networks, which are reminiscent of the filament networks close to the outer plasma membrane of cells. These new types of biomimetic membranes have a large potential for applications as drug delivery systems.

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In addition to the soft and flexible assemblies discussed so far, biomimetic research has also produced hard materials in the form of biomimetic minerals. These minerals are typically built up from rather simple building blocks such as hydroxyl apatite or calcium carbonate. However, biological cells are able to control the detailed morphology of these minerals. As a result, the same building block such as hydroxyl apatite leads to rather different materials such as teeth and bone. It has been recently shown that such processes can be mimicked, to a certain extent, by growing the minerals in the presence of organic additives such as synthetic copolymers in aqueous solution.

(c) Recent developments: complex architectures

The next level of complexity consists in supramolecular architectures which incorporate different types of building blocks and/or which contain different types of supramolecular assemblies.

Several attempts have been made to built up complex architectures consisting of rodlike filaments within membrane compartments. It has been demonstrated that both actin filaments and microtubules can be polymerized within lipid vesicles. This can be directly observed in the optical microscope since the growing filaments induce morphological transformations of the vesicles. In the case of actin, two different procedures have been realized. One of these procedures led to shells, which are reminiscent of the cytoskeleton cortex, the other to protrusions, which resemble microvilli.

The layer-by-layer construction of polyelectrolyte multilayers makes it possible to incorporate layers of different species of polyelectrolytes and/or of other types of colloids. In this way, one can construct complex multilayers, which represent multifunctional interfaces.

Complex architectures may also be constructed using chemically structured surfaces. Indeed, the multifunctional interfaces of biomembranes arise from the lateral organization of these membranes into specialized membrane domains. New techniques have been developed which make it possible to chemically structure solid surface on the nanometre scale. These structured surfaces can be used to build up supramolecular architectures with a defined lateral organization.

2.4.3. Future Perspectives

There are many challenges for biomimetics on the supramolecular (or colloidal) scale. One important and general goal is to gain *improved control* over the structure formation and over the morphology of the supramolecular assemblies. In particular, one would like to construct biomimetic systems, which undergo reversible transformations and, thus, can be switched forward and backward between different types of assemblies or between different types of morphologies. Likewise, one would like to incorporate such reorganisable structures as subsystems into larger architectures.

Future research projects, which will lead to such an improved control include:

- Construction of spatial patterns of filaments. This could be achieved, e.g., by anchorage to chemically structured substrates;
- Controlled assembly and *disassembly* of filaments;
- Lateral organization of membranes into well-defined domains;
- Biomimetic recognition systems or biosensors based on immobilized membranes;
- Controlled formation of membrane buds mimicking the cellular processes of endocytosis and exocytosis;
- Model systems for the fusion of membranes;
- Minerals with defined morphologies on the nanometre scale;
- Biomimetic transport systems based on filaments and molecular motors in open and closed compartments. The latter type of systems is inspired by the directed transport as found in the axons of nerve cells, see Fig. 2.5.

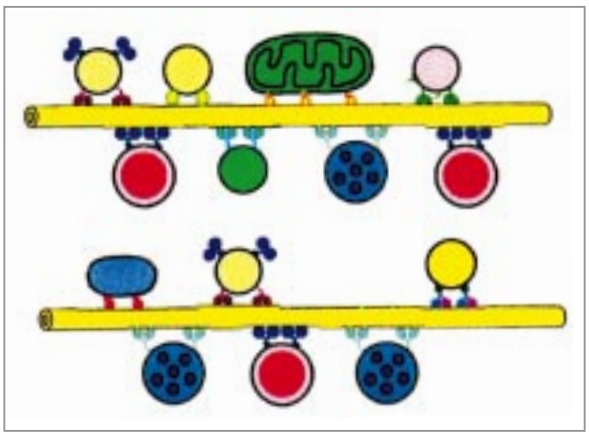

Fig. 2.5. All microtubule filaments within an axon have the same orientation. Cytoskeletal motors (indicated by small "feet") are responsible for the directed transport of various particles along these filaments.

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A more ambitious long-term goal would be to combine biomimetic sensors and motors in order to get model systems for biological signal transduction. Thus, one may envisage autonomous nanorobots, which receive physical or chemical signals from their environment and respond to this information with some "action".

In the very long run, research on biomimetic systems could lead to construction kits by which one can create artificial cells. At present, this vision must still be regarded as science fiction.

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2.5. Materials Science in Catalysis

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2.5.1. Introduction

Catalysis is the technology, which allows to increase the rate and selectivity of a chemical reaction by a substance, which is, to a first approximation, not consumed during the reaction. Catalysis has a major impact in the chemical and related industries, as all chemicals, which are raw or intermediate products for other industries are obtained using this technology. The overall catalyst market is around 10 billion € (Fig. 2.6), the revenue generated by processes using catalysts is difficult to estimate, but exceeds the catalyst market probably by factor between 100 and 1000, i.e. is somewhere between 1.000 and 10.000 billion €. In addition, catalytic processes are also ecologically superior to non-catalytic processes in that they typically consume less raw materials and energy. Even slight improvements in catalyst performance can translate to big savings in raw materials and energy in large-scale processes, since there are many base chemicals, which are produced via catalytic routes in volumes exceeding 1 million metric tons per year.

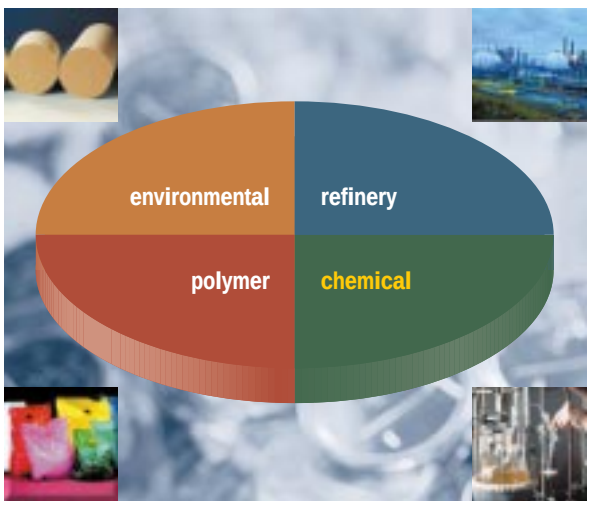

Fig. 2.6. Catalyst market (total around 10 billion €) and division into different application fields.

A large potential for catalysis exists in fine chemicals production, where many conversions are still carried out stoichiometrically with large amounts of waste being produced or toxic reaction routes (chlorinated hydrocarbons as intermediates) being technological practice. Replacing such reactions with catalytic steps would lead to tremendous improvements.

Catalytic reactions are not only important in the chemical industries, but also in other sectors of the European economy. Table 2.1. gives examples for the importance of catalysis in different fields and also addresses some of the challenges, which still exist.

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2.5.2. State of the Art

Since materials science deals with solids, this section will primarily focus on conversions, which are catalyzed by solid catalysts ("heterogeneous catalysis"). This corresponds to the fact that the majority of the industrially used catalytic conversions are heterogeneously catalyzed reactions. However, homogeneous catalysis and biocatalysis are increasing in importance, and one of the trends in catalysis research is the merging of these different fields. It can thus be expected, that homogeneous and biocatalytic reactions will also be increasingly applied in industry.

Scientifically, catalysis might on a first glance appear to be a mature science: Based on empirical knowledge acquired over decades, scientists and practitioners have guidelines how to select a catalyst for a given reaction – at least for some generic classes of reactions. Over the last years, this toolbox has been supplemented by the advent of high throughput experimentation in catalysis research, which accelerates the rate at which experiments can be performed, and expands the parameter space of conditions and catalyst compositions, which can be explored.

The empirical knowledge base has, however, reached its limits for many applications, as decades of research have to be invested for a marginal improvement of the performance (e.g. in selective oxidation catalysis).

ious techniques developed to study elementary steps in homogeneously catalyzed reactions. Also the theoretical treatment of catalysts and catalysis is developing fast. It is now possible to calculate interaction energies of molecules with model surfaces, in some cases even reaction pathways have been predicted (Fig. 2.7).

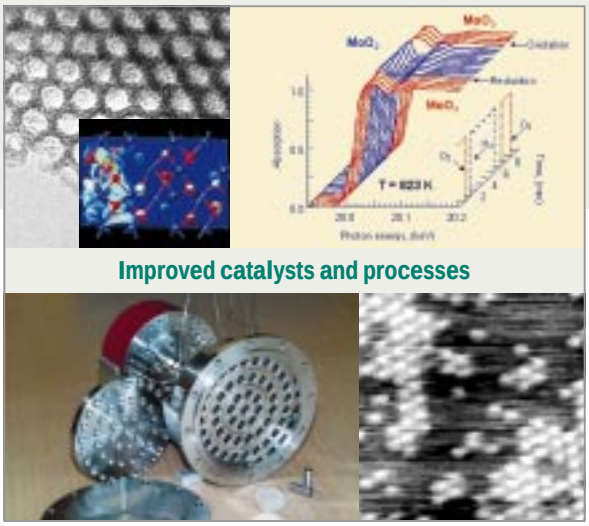

Fig. 2.7. State of the art in catalysis research. Starting from upper left, then going clockwise: Modelling of solid-reactant interaction (MSI), regular porous silica with a surface area of 800 m^2/g (MPI für Kohlenforschung), *in situ* EXAFS spectra of MoO_3 catalyst (Fritz-Haber-Institut), *in situ* atomic force microscopy of adsorbed oxygen (Fritz-Haber Institut), 49 channel high throughput reactor for accelerated catalytic testing (MPI für Kohlenforschung).

Industry segment	Application example	Exemplary problem
Chemical	Various	Small alkane oxyfunctionalization
Petroleum	Cracking, reforming, alkylation etc.	Replacing sulfuric acid in alklyation
Energy	Selective catalytic reduction of NO_x, catalytic combustion, fuel cell	NO_x decomposition, high temperature stable combustion catalysts, photochemical hydrogen generation
• Automotive	Fuel cell, $DeNO_x$	Fuel processor for fuel cell, lean NO_x
• Electronics	Fuel cell for mobile applications	Fuel cell catalysts

Table 2.1. Catalytic reactions in various application fields.

Going beyond this heuristic knowledge, an understanding of the catalytic action and the principal steps in several important reactions has been achieved. There are tools available for studying well defined model systems, such as the surface science techniques to investigate single crystal surfaces under high vacuum conditions or the var-

However, although a high degree of knowledge in catalysis has been achieved, there are still many problems of a fundamental nature unsolved. There is, for example, no verified understanding of the local structural and electronic requirements of a surface on a general basis. Fundamental work to solve these problems are the long-term

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trends in catalysis research, and these problems and trends will be described in the following.

2.5.3. Expected Breakthroughs

The ultimate vision of catalysis research is the ability to *de novo*-design a catalyst for any given reaction (Fig. 2.8). There are many "dream reactions" which so far cannot be performed on a commercial scale or even on the laboratory scale, although these reactions should in principle be possible. Catalytic routes could make such reactions possible, if design principles for catalysts were available. This goal will not be reached on a short time scale of several years but is probably still decades away. In the meantime, high throughput experimentation will be an important transition technology to discover novel catalysts for burning catalytic problems which need to be solved, for instance to allow the introduction of a fuel cell based transportation system.

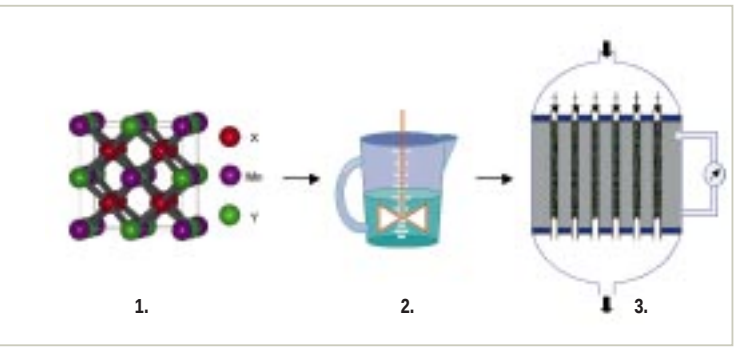

Fig. 2.8. Ultimate goal in catalysis research: 1. Calculate catalyst requirements for a desired transformation from first principles. 2. Rationally synthesize catalyst with calculated characteristics, 3. Use in catalytic process.

To approach the ultimate goal of a catalyst design, fundamental coordinated research is necessary, since isolated activities are mostly focused on special reactions from which only limited generic information can be derived. Typically, research in this field is highly interdisciplinary, since chemists, physicists, theoreticians, and engineers are necessary to tackle the fundamental questions from all directions. On the way to a catalyst design, methodologies will have to be developed which will not only help to advance the field of catalysis, but will also have effects in other, related fields of research. In addition, it can be expected, that from some exemplary catalytic problems, which are chosen to develop the methods, breakthrough discoveries for specific catalytic reactions will be made.

2.5.4. Roadmap of European Catalysis Research

Catalysis science is, despite its interdisciplinary character, usually split between physical chemistry, inorganic chemistry and chemical engineering, which is not a uniting discipline for catalysis, as e.g. in the U.S.

Industrial catalysis research is occluded behind huge walls to protect intellectual property. Today's catalysis technology is predominantly based upon empirical findings, and existing plants contain many proprietary key features essential for commercial success. It is almost impossible to do process-relevant research in co-operative structures.

The progress of fundamental knowledge in the last decade allows, however, to define a few key actions to be taken in order to move forward in a faster way in this fundamental technology. The turnover times in catalysis technology is very long with 15 to 20 years and the readiness of industrial users for new technology is very limited which results from the enormous risks related with the huge capital investments and the technological and safety uncertainties associated with large scale production facilities. All this could be tremendously more efficient and development benefits could be brought to bear on economics and environment much faster, if the development basis of new catalysis technology would be more rational and more transparent than the present empirical search.

The following description of key areas of possible European research engagement is based upon the idea to focus efforts on generically relevant issues and to abstain from supporting individual reaction types by again empirical optimization strategies.

(a) Bridging the gaps between model studies and real world catalysis

There are well-developed tools available to study catalytic reactions with surface science techniques on model surfaces. There are also some techniques, which are suitable for an *in situ* analysis of the catalyst under process conditions. However, the gaps between these two approaches – the so-called pressure gap and the materials gap – are substantial. It is generally impossible to transfer or extrapolate results obtained under UHV conditions to the catalytic reaction under process conditions, because the partial pressures of the reagents and thus their internal interactions differ by many orders of magnitude, and, possibly more severe, the catalytic surfaces are not identical under UHV and at higher pressures.

It appears that for many catalytic reactions the real structures of the catalysts, i.e. their defects, particle shapes and

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other properties, are most decisive. This, however, will be difficult to mimic in a model system. Great efforts are therefore needed to bridge this gap between model studies and real world catalysts, to analyse the real structures of solids and to develop more powerful *in situ* techniques. To study catalytic reactions under process conditions in order to understand the influence of these factors on the performance of a catalyst. These allow to study catalytic reactions under process conditions in order to understand the influence of the reaction conditions on the performance of catalysts.

Such studies, especially the analysis and the understanding of the defect structure of solids, are not only important in catalysis research but have far wider implications, since for almost any material the defect structure could determine – or at least influence – the performance of the material in applications.

(b) Understanding catalytic reactions on an atomic level

For a true understanding of catalytic reactions, means have to be developed to study such reactions on the atomic scale and to describe the processes on catalytic surfaces theoretically from first principles. First steps in this direction have been taken, and reaction rates measured by direct observation with atomic resolution (Fig. 2.9) correlate well with macroscopically determined reaction rates. However, these successes are so far limited to simple reactions on model metal surfaces.

Parallel to the development in experimental techniques, answers to the nature of the elementary steps in catalytic reactions will come from high-end *ab initio* theory. Such theory has reached a state, where close interaction between theoreticians and experimentalists is fruitful for both sides. First calculations on the course of chemical reactions on surfaces have been performed and provide meaningful data. Invaluable are the contributions of theory in predicting stability and dynamics of catalyst surfaces (oxides) and the interactions of these surfaces with the gas phase (dynamics of termination, sub-surface compound formation).

Also here fundamental understanding will not only be important in catalysis, but the methods developed to study surface reactions on the atomic scale will bear influence on many other fields of materials science.

(c) Development of rational synthesis strategies for catalysts

Understanding of elementary steps in catalytic reactions is only one prerequisite for a catalyst design. Even if one knows exactly what the composition of a catalyst should be and what real structure it should have, there is at present no rational synthesis strategy available, which could be used to develop a preparative route to a complex solid on a large scale. Today, solids formation is only poorly understood on an atomic level, and – as in the development of catalysts nowadays – the synthesis of solids with desired structure and properties is largely empirically driven. Therefore techniques to analyze the steps leading to solids formation on an atomic scale need to be developed, so that details of nucleation and solids growth can be understood. A full integration of experimental and theoretical approaches is necessary to this means.

Since modern catalysts are typically multicomponent systems, not only nucleation and growth of single phases need to be understood, but also the development of such complex solids. For instance, in the case of supported catalysts, the development of the real structure and the interaction of support and solid are only sketchily understood, although this drastically influences the performance of a catalyst.

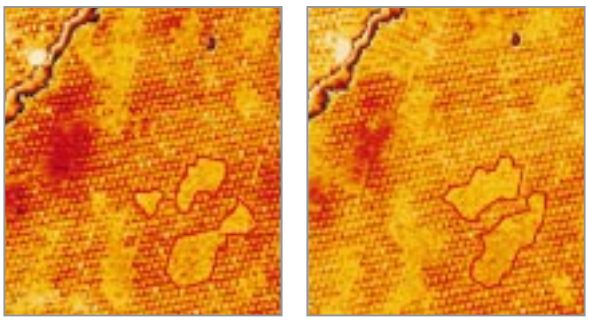

Fig. 2.9. Scanning tunneling microscopy during the reaction of CO and O_2 on Pt(111). The lines show the borders between oxygen and CO domains. Appr. 100 s between pictures (Fritz-Haber Institut).

As in the other research fields, which are important in catalysis research, also the development of synthesis strategies for solids has far reaching implications in other fields of materials science. The solids properties, which need to be adjusted during the solids synthesis, and thus controlled by nucleation and growth, are also important in the production of pigments, building materials, and even the production of pharmaceuticals.

(d) Integration of heterogeneous, homogeneous and biocatalysis

Industrial catalysis is nowadays dominated by heterogeneous catalysis. There are reasons for this, such as often better stability of solid catalysts and easier separation of catalyst and product. However, homogeneous catalysts are generally better understood on the atomic level, and heterogenization of homogeneous catalysts could help to solve

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some of the problems typically associated with homogeneous catalysis. In addition, homogeneous catalysts are much superior in enantioselective conversions. This advantage is even more pronounced in biocatalysts, which are amongst the most active and selective catalysts known. In addition, they typically operate under very mild conditions, such as ambient pressure and only slightly elevated temperatures. Moreover, they can be very efficiently optimized for specific reactions by the novel techniques of directed evolution. First steps to overcome the barriers between the different branches of catalysis have been taken, for example, in mimicking enzyme active centres in the environment of zeolites or by modelling enzymes with organometallic model complexes.

A true holistic approach towards catalysis cannot maintain the traditional separation between the three branches of catalysis, which only very moderately overlap at present. Fundamentally, the mode of action of homogeneous, heterogeneous and biocatalysts should be identically. On the atomic level all kinds of catalysis are governed by the same principles, and a true understanding of the nature of catalytic conversions will lead to a vanishing of the borderlines between these subfields of catalysis.

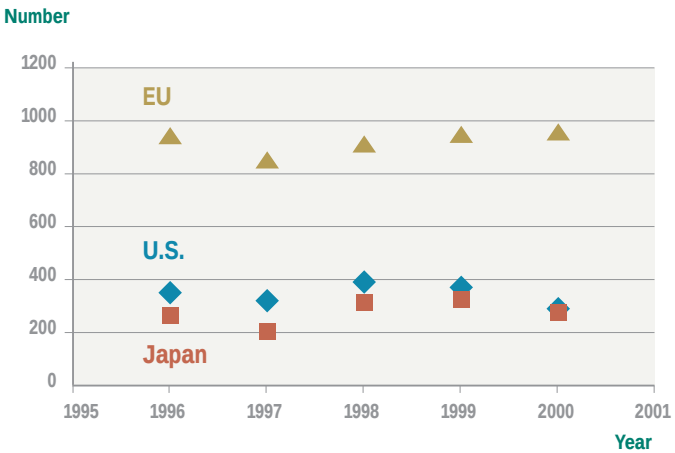

Fig. 2.10. Number of publications in catalysis journals for the EU, U.S. and Japan.

2.5.5. Position of Europe Compared to the U.S. and Japan

Catalysis research in Europe is typically very strong compared to the rest of the world (Fig. 2.10). In many fields of catalysis European companies and research groups are leading in the world, and this does not only hold for one or two European countries, but basically all over Europe. The present trends seem to be a decreasing activity in catalysis research in U.S., since most of the funding is channeled into projects including words with the prefixes “bio” or “-nano”. This has already led to a situation, where many American companies look towards Europe when they want to hire catalysis specialists. Due to the limited number of students entering universities to study sciences, the competition for qualified chemists, physicists and engineers will become stronger, and even now European companies are facing a severe shortage in well-trained scientists in the field of catalysis. The situation with respect to Japan and East Asia is different, since in these countries increased activity in catalysis research can be identified.

The leading position of Europe in this field needs to be maintained and strengthened, since catalysis will remain to play a key role in the development of more economical and environmentally benign processes. With respect to the materials basis of our economy, Europe can only be competitive, if better processes – which in the chemical and related industries almost always means catalytic processes – are constantly being developed, since many of the mature processes can be operated in developing countries more economically.

2.5.6. Structure and Organization of European Catalysis Research

The academic catalysis research in Europe is organized in many countries in national virtual networks. The representing learned societies in Europe have founded EFCATS, the European Federation of Catalysis Societies which is an active body and which organizes the European catalysis conference, having matured to a world-class event.

The industrial interest groups of producers and users of catalysis technology are also organized, in NICE, the Network of Industries using Catalysis in Europe, an organization covering all major industrial players. Its current activities lie in the identification of needs and challenges for research, done usually in specialized workshops complementing academic conference topics.

Both organizations are stable institutions, which could and should play a role in organizing future European catalysis research. A close co-operation of both bodies can ensure the direction of activities according to the needs of industry. Only then the technological achievements can be brought to bear in European societies, as unlike in other fields of technology, catalysis and the production of chemicals and energy are characteristically large-scale technologies with limited room for small industrial activities.

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2.5.7. Preconditions for EC Actions in Catalysis

First, it must be realized that the technology of catalysis is a fundamental and key technology to a wide range of industries as all chemicals and most functional materials are produced by catalysis.

Second, it is important that from a thermodynamic point of view the overall industrial efficiency in producing the desired materials is about 50%. This gives an impression of the potential for improvements of existing technologies into directions of ecological and sustainable production.

The revolution in automotive technology which we may face with hydrogen-based traction systems requires massive developments and quantum leaps in catalysis technology, both on the sides of producing hydrogen-storage fuel systems (artificial petrol, methanol, ammonia) and in the on-board technologies of fuel processing and electrocatalysis.

2.5.8. Actions Suggested for the EC Framework

With these perspectives it seems essential to concentrate research efforts on the creation of a development platform and not to disperse the resources in the solution of specific problems with strategies from the past.

The construction of an advanced technology platform for catalyst development requires basic research with a perspective of about 10 years, consisting of three major components. Integration of the traditional fields of chemical engineering, synthetic chemistry and physical engineering is a further prerequisite for success in this field. The necessary components are:

- Evolution of high throughput technologies in their respective fields (different for molecular and solid state catalysis) into enabling technologies applicable by industry on a routine basis. To achieve this, a suite of instrumentation for synthesis and testing of catalysts as well as a suite of high throughput characterization tools needs to be created. Information technology and design tools for experiment strategies are essential ingredients to such a technology, which require equal attention as hardware developments.

- Construction of a suite of methods allowing efficiently to functionally characterize existing catalysts in order to create a secure knowledge base for novel developments. Large-scale facility access as well as creation of equipment for *in situ* functional analysis are pressing hardware requirements. Equally important is the broad integration of theory and computer modelling into such a project, which should be done on an "on-the-fly" basis and not in the way that theory explains previously obtained experimental findings. This new co-operation between theory and *in situ* experimentation is only possible due to the enormous progress in both areas over the last five years.

- Development of methods for the rational synthesis of solids. Even if the requirements for a new catalyst are clear, it is nowadays not possible to devise a rational synthetic route to create it. Concurrently with the activities in the other fields basic research into the understanding of the elementary processes during catalyst formation is mandatory to achieve full control over the properties of the final material.

The most suitable framework for this platform is clearly the creation of networks using the existing, but underequipped and uncoordinated research infrastructure in many European countries. Significant investments in equipment are essential as well as the creation of a flexible organizational structure, which should be built on the existing organizational infrastructure mentioned above (Fig. 2.11).

2.5.9. Roles of Academia and Industry

The chemical and application industries are the recipients of all development efforts in catalysis. Industry should thus have a major influence in the evolution of the platform, which is designed to be used by them.

A big obstacle in this endeavor is the secrecy consciousness of chemical industry, which is extremely reluctant in disclosing or even undergoing any risk of giving insight into any details of their production technology. For this reason it is intrinsically problematic to bring industry into efficient co-operations close to production-related problems. In the past, frequently technologically less relevant projects were pursued in co-operative activities, which wasted thus significant resources to protect the relevant information from disclosure.

It seems thus adequate to organize future networks in such a way that industry takes the strategic lead but does only contribute to the operations in the framework of pre-competitive actions pursued in their own laboratories. Industrial companies are essentially required as partners in future frameworks but without the obligation to produce

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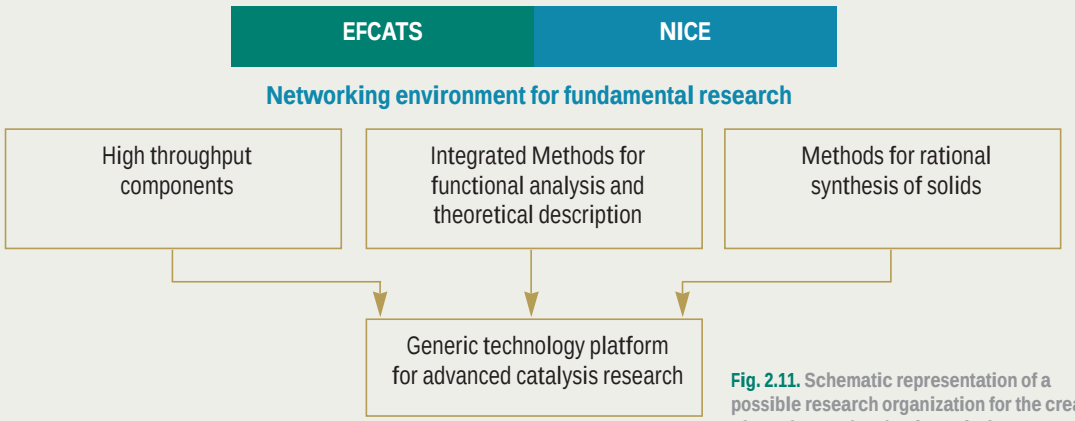

Fig. 2.11. Schematic representation of a possible research organization for the creation of an advanced technology platform.

commercially relevant results. The whole effort should remain pre-competitive and be directed towards the creation of technology, which is later used by industry outside the development networks. Success or failure of such activities may be measured by the documented technology transfer and not by the difficult-to-assess direct commercial value of a particular development.

2.6. Optical Properties of Materials: "Harnessing Light" [1] through Novel Materials

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2.6.1. Scope of Optical Materials

Optics is defined as "the field of science and engineering encompassing the physical phenomena and technologies associated with the generation, transmission, manipulation, detection, and utilization of light. It extends on both sides of the visible part of the electromagnetic spectrum as far as the same concepts apply." The very definition of all functions assigned to optics show that the progress of optical science and technology is closely determined by progress in optical materials.

Optical materials are developing rapidly in response to expected improvement in technological performance. Indeed, the sole field of optical telecommunications by itself generates a high level of demand with tough requirements to continue its progression along the optical version of "Moore's law" under which the capacity of one single fibre has been increasing by 33% every year since the mid 1970-ies. In addition, hardware for information science and technology in general, as well as energy, environment, and consumer products, are further application areas for the development of novel optical materials. All classes of materials, including in particular semiconductors, dielectric crystals and organics are relevant. In this document, we review challenges faced by optical materials research by the required function: light emission, nonlinear functions in a broad sense including modulation and detection, or plain passive propagation and transmission.

1) "Harnessing light ist the title of a recent report on the potential of optics by the U.S. National Research Council, 1998.

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In spite of outstanding existing skills in Europe and the U.S., Japan, in some case in association with pioneers of the field from the UK, has recently taken a lead in organic electro-optics with some first commercial product. Also, a Japanese company has also introduced blue solid state lasers on the market. The U.S. have strong consortia on guided wave optics, infrared materials, vertical emitting lasers, and have been successful in pro-actively promoting materials technologies for future micro-electronics, e.g. involving X-ray imaging lithography. However, in a tough competition, European research is present on essentially all major topics, such as materials for telecommunication sources, fibres and planar optics, organic materials, photorefractive crystals, novel laser materials. EC funded consortia have included optical materials but have not yet fully exploited the possibility of giving an European dimension to optical material research. Yet, national initiatives have been successful and can be used to that end; to cite but a few, in France, "groupements de recherche" have benefited research on laser materials, nonlinear optical materials, photonic bandgap structures and microcavities; essential progress has been pioneered in the UK on photonic crystal fibres, laser amplifiers, and in Germany on surface emitting lasers, among others.

2.6.2. State of the Art

(a) Light sources

i) Laser diodes and light emitting diodes More than half of the multibillion market of compound semiconductors is devoted to light sources. Present challenges include bandwidth extension, spatial and spectral control. In addition to efficient pumps for telecommunication fibre lasers used in long haul transmission, telecommunication applications require wavelength control for dense wavelengths division multiplexing with hundredths of independent channels being carried in the telecommunication bandwidth, that would ideally need to be extended to 1.2 µm through 1.65 µm with good temperature behaviour, extremely high spectral stability and accuracy, and high energy efficiency. Increasing the density of optical memories demands shorter wavelengths – blue diodes at 430 nm are expected on the market very soon from Japanese sources but significant increase in performance and further wavelength decrease are still required. Combined blue, green and red light emitting diodes or laser diodes may revolutionize lighting technologies with significant energy savings arising from better conversion of electrical to optical energy. Laser diode pumping of very high energy short pulses in the picosecond and femtosecond regimes are required for plasma research, with application to extreme ultraviolet and soft X-ray sources of industrial interest, e.g. for lithography.

Most progress on laser diodes derives from innovative band gap engineering and tighter fabrication control of heterostructure semiconductors relying on molecular beam epitaxy or metal-organic chemical vapour deposition; industrial processes, though, would ideally benefit from improved liquid phase epitaxy.

ii) Solid state lasers, parametric oscillators Dielectric crystal lasers, known as solid state lasers, complement diode lasers by offering better spatial beam profile properties and a very broad spectral range from the mid ultra-violet to the mid-infrared needed for applications in information technology, sensors, and environmental monitoring. They are expected to totally replace gas lasers and dye lasers in the coming few years, offering more reliable consumer friendly operation in more compact units with equally good beam quality. When a good spectral match is available, diode laser pumping of solid state lasers offers the most compact and energy efficient solution. Yet, the classic titanium doped sapphire crystal, that offers unique performance in ultrashort pulse generation, cannot yet be efficiently pumped by laser diodes. One competitive domain of research is therefore the identification of potential laser crystals for diode pumping and ultra short pulse generation, such as ytterbium ion doped materials that have progressed significantly lately.

The generation of controlled frequency beams through non-linear effects in a suitably pumped non-linear crystal, known as parametric oscillation, is one of the latest paradigm in coherent sources, offering the broadest range of spectral tenability.

iii) Fibre amplifiers and lasers The introduction of optical fibre doping with rare earth for amplification and for fibre lasers was a vital change in telecommunication concepts. Improved gain control over a broader spectral range together with dispersion engineering and non-linear propagation control as well as application of these components outside the communication area are now research challenges. High power carried by monomode fibres is required for efficient Raman amplifiers.

(b) Materials for nonlinear optics and light detection

In a broad sense, nonlinear optics includes all effects whereby an electromagnetic field affects the propagation of another electromagnetic fields. This usually occurs through modulation by the control field of the refractive index "seen" by the probe field, thus affecting beam propagation phenomena such as convergence, diffraction, or absorption. The control field may be of any spectral domain from low frequency "electronic" signals to "optical" waves. For example, nonlinear optical effects have become domi-

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nant together with dispersion control in designing long haul fibre transmission lines, and the optical control of light pulses in telecommunication signals is of course vital for the challenge of all-optical switching. Storage materials showing such properties as nonlinear recording by second harmonic generation, high index modulation recording, and 3D patterning are essential and urgently needed for future mass storage technologies. A wide open gap is the present lack of materials for short term, fast access storage devices and shift-registers.

i) Semiconductors Heterostructures and in general band-gap engineering has been essential for the fast modulation and detection of light over an extended spectral bandwidth. Present challenges include the bandwidth extension beyond 40 Gbits/s per channel and direct microwave modulation optical signals.

ii) Organic compounds While unlimited engineering flexibility and direct control of molecular orbitals for modulation bandwidths in the 100 Gbits/s range in polymers have attracted interest for years, stability and process control have proved hard to achieve. Recent breakthrough on so-called "conjugated" polymers showing a gap for charge carriers and luminescence upon recombination open clear hopes of popular commercial applications for large, relatively inexpensive soft films used as light sources and displays. Low cost is also a major issue in end-user access of optical communication ("fibre to the home").

Doping controls conductivity and determines, among others, structures suitable as electrode materials. Organic light sources have been extensively investigated in European research laboratories but industrial applications seem to be somewhat lagging behind Japanese achievements. Excitation, orientation and relaxation mechanisms, synthesis of suitably pure chemical bases, stable dye grafting compatible with the required nonlinear effects are still wide open for research and emerging applications. Stability is mainly determined by purity, the influence of oxygen and photodegradation.

Liquid crystals have been famous and successful for years for display, but progress is still expected in large, bright display applications as well as in relatively fast (submillisecond) control of large screens with potential application to motionless "spatial switching" fabrics.

iii) Photorefractive materials So-called photorefractive materials exhibit a noteworthy specific property: control light beams induce an internal photoelectronic effects and photocarriers are trapped in defect sites, creating a space charge field that in turn electro-optically modulates the refractive index. Photorefractive materials open new perspectives for the development of laser mode control in space and time, and therefore higher beam quality and higher brightness. Some photorefractive crystals have been successfully inserted into industrial systems and can now be fabricated to suit application driven specifications, e.g. for vibration and deformation sensors. Further material optimization is still needed for others, with potential application in such areas as environmental monitoring (Fig. 2.12). Again, a broader spectral bandwidth, together with temperature stability, are major materials sciences challenges.

iv) Artificial non linear materials and nanomaterials A beautiful achievement during the recent years has been the control of efficient frequency doubling by anisotropy modulation along the propagation axis to secure phase matching between the illuminating and frequency doubled waves. Such synthetic phase matching materials are now being developed in thin films as well as in bulk dielectric and semiconductor materials. "Poling", or electric field induced anisotropy, confers new nonlinear properties to some inexpensive materials as glasses.

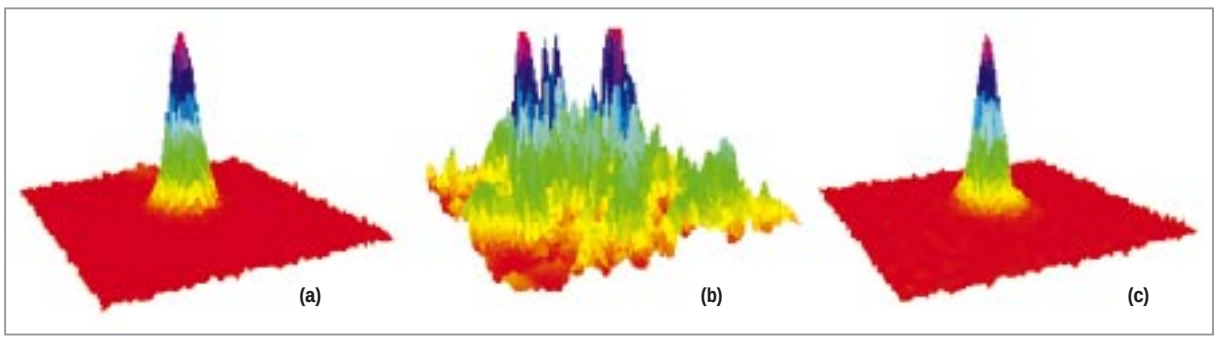

Fig. 2.12. Restoration of a Gaussian laser beam (a) after degradation by a diffusing medium (b) such as a turbulent atmosphere, an inhomogeneous optical material or even a strongly diffusing biological sample, can be achieved by four wave mixing in a non-linear "photorefractive" material (c).

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Another form of artificial materials results from incorporating nanocrystallites into suitable matrices. Such so-called nanomaterials offer fundamentally new properties: quantum confinement, plasmons bands, 2D and 3D self-organization, enhanced scattering (resonant Raman scattering, fluorescence), and magnetic properties. Important efforts have been devoted recently to size uniformity of the nanocrystallites incorporated in glasses, polymers, sol-gels and others. Potential outcome includes ultra-fast and high nonlinearities opening the way to optical limiting, optical storage properties, and light probes for imaging, including in biological applications.

(c) Passive optical materials

i) Glasses Low temperature fabrication of glassy materials using the sol-gel process, as already mentioned for its potential in nonlinear optics, has already significantly impacted thin film deposition processes for consumer applications and could affect bulk material fabrication if shrinking and water ejection could be avoided. Superpolishing techniques on glass has reached sub angstrom smoothness down to micrometre scales, and requirements for X- ray optics imply a further tenfold improvement.

Heavy oxide and chalcogenide and halide glasses are opening new spectral windows in the mid and far infrared. Inexpensive mouldable infrared materials have scarcely started to appear but would offer sizeable market opportunities. Fluoride glasses for low loss transmission in the mid-infrared would be particularly valuable for application. High power laser beam transport requires specific glasses and fibre end coatings.

Ophthalmic optics may still benefit from progress on organic and inorganic glasses: anti scratch, anti reflection, anti halo, rapid photochromic glasses are desired and require more work on material chemistry.

ii) Mesoscopic patterning of optical materials Almost all optical materials are "synthetic" materials, as they require sophisticated elaboration processes. "Artificial" materials in addition combine mesoscopic structures smaller than the optical wavelength that confers optical properties different from the bulk and strongly dependent on detailed microstructure. The simplest case is thin film deposition for reflection control, where loss control down to less than one part in a million is still a challenge, for example for high accuracy interferometry and for high power laser applications. Multilayers providing high reflection in the extreme ultraviolet domain are a challenge for year 2008 nanolithography with a significant impact on the microelectronics market: Europe must remain in the competition and has all industrial and academic partners required to do so. 2D and 3D microstructures give rise to the so-called "photonic bandgap materials" (Fig. 2.13), that offer a very nice combination of basic science research opportunities and very large application potential for the fabrication of highly integrated photonic circuits, firstly in a planar guided wave configuration and in the longer term perhaps in 3D space.

Full 3D control of optical propagation and nonlinearities is an ultimate challenge for research in optical materials, micro-optics and optical information technologies. Electronic ink and diffuse displays are typical examples of still wide open research that would clearly require both novel materials and nanometre scale patterning.

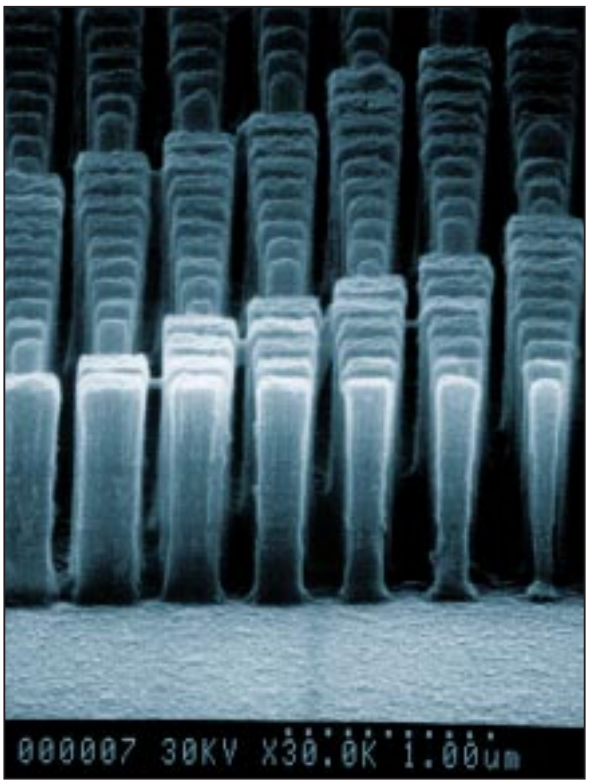

Fig. 2.13. «Effective index» behaviour results from subwavelength patterning of transparent materials and offers some unprecedented possibilities for diffractive optics and micro-optical systems.

2.6.3. Challenges and Expected Breakthroughs: Research Priorities

Here we suggest some possible priorities that may be used for an European Materials Framework programme in relation with the three categories of materials functions that were developed in the preceding section:

- Sources: reduce the cost of high average power, high beam quality sources (typical values: 10W average pow-

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er and M2 factor below 1.5). Develop materials that will deliver plug efficiency over 30% white light. Develop semiconductor lasers that will directly produce high power, high beam quality. Develop all-fibre laser covering the whole spectral range of interest to telecommunications. Develop fibre lasers for mid-IR range environment monitoring.

- Active materials: develop stable materials for 100 Gbits/s modulation and beyond. Develop self-luminous organic displays that can be developed into large matrices. Demonstrate active materials improving vision through fog through phase conjugation. Demonstrate active patterning of electro-optic switches in a two-dimensional photonic bandgap material.
- Passive materials: demonstrate less than .1 dB/cm losses in a two-dimensional photonic bandgap material. Obtain record reflection factor over whole vacuum UV and extreme UV range for space and microlithography applications (120 down to 10 nm wavelength). Propose material solutions for reflecting multilayers below 10 nm. Develop fibres for high power laser transport at all wavelengths of interest to laser machining, welding and deposition.

2.7. Magnetic Materials

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2.7.1. Introduction

Never before has our daily life and environment been so significantly dependent on materials with outstanding magnetic properties. Modern life is today in many aspects an automated world which uses ferro- and ferrimagnetic materials in nearly all important technical fields as, e.g., electrical power, mechanical power, high-power electromotors, miniature motors, computer technique, magnetic high-density recording, telecommunication, navigation, aviation and space operations, automation micromechanics, medicine, sensor techniques, magnetocaloric refrigeration, materials testing and household applications.

Recent developments in the field of exchange coupled thin film systems and the use of new techniques for the development of nanocrystalline (nc) magnetic materials have initiated numerous activities for the development of advanced magnetic devices for energy transfer, for high-power and miniature electro motors, for medical applications and for the sensor and magnetic recording industry, nowadays known as magnetoelectronics. Most of the progress achieved so far was due to the discovery of new materials with extremely low (0.1 J/m^3) or extremely large magnetocrystalline anisotropy (10^7 J/m^3) as well as to the tailoring of high coercivities, H_C, which are determined by the microstructure and vary between 0.1 A/m to several MA/m. Further progress in these fields is possible if we succeed to develop materials with optimal *property spectra* where magnetic, electrical, mechanical, corrosive and thermal properties are optimized simultaneously. These advanced magnetic materials also result in considerable energy savings and in the case of magnetocaloric refrigerators, i.e., refrigeration without the use of chlorofluoro-carbons, the destructive impact on the ozone layer is avoided.

2.7.2. State of the Art

Here only a brief review of advanced magnetic materials used today will be given. These materials in general have a nanocrystalline (nc) structure or, in the case of thin films, at least one dimension is in the nanometre scale.

- High-permeability nc-materials based on Fe_3Si with additives of Cu, Nb, Zr, B (Finemet) achieve permeabilities up to $10^5 - 10^6$.
- High-coercivity nc-magnets based on $Nd_2Fe_{14}B$ and CoSm alloys with coercive fields of 1.5 T for NdFeB and up to 3.5 T for Sm_2Co_{17}-based magnets. Maximum en-

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ergy products of technical magnets of 450 kJ/m^3 have been achieved. The development of composite materials has started.

- Giant-magnetostrictive nc-magnets with $\lambda \geq 10^{-3}$ based on (FeTbDy)-alloys for micromechanic applications.
- Giant-magnetoresistive (GMR) thin film systems for read heads with magnetoresistances $\Delta R/R > 50\%$ and high permeability. Examples of multilayer systems are CoFe/Cu or Fe/Cr. Systems of GMR films are used to develop nonvolatile "Magnetic Random Access Memories" (MRAM).
- Colossal-magnetoresistive films of LaSr- and LaCa-Manganites with $\Delta R/R > 100\%$.
- Giant-magnetocaloric refrigerator material as $Gd_5(Si_2Ge_2)$ with $\Delta T > 20$ K effects.
- Molecular magnets based on metal-organic compounds based on hexafluoroacetylacetonat or tetracyanomethylen.
- Self-organized superlattices of ferromagnetic nanoparticles of FePt or FeCo for high-density recording (Tbit/inch^2).
- Computational solid state physics for the calculation of intrinsic material properties and phase diagrams.
- Computational micromagnetism of magnetic ground states and the dynamics of magnetization processes in nc materials, thin platelets and small particles.

2.7.3. Future Visions

Magnetic materials used presently in general are characterized by *one* outstanding property as, e.g., high permeability, high coercivity or high remanence. For technical application, however, it is a pre-requisite that a whole *spectrum of properties* has to be optimized. In so far the development of materials with optimal magnetic, electrical, mechanical, anticorrosive and thermal properties as well as low hysteresis losses is one of the main topics in this field.

Concerning the different types of materials outlined in Sect.2.7.2 it is obvious that all of them are strongly dependent not only on intrinsic material parameters as spontaneous magnetization, J_S, magnetocrystalline anisotropy, K_1, magnetostriction, λ_S, and Curie temperature, T_C, but also on the special types of microstructures. Actually the deviations from the ideal lattice in many cases are responsible for certain outstanding properties. In particular nanocrystalline microstructures and composite materials allow a wide variation of microstructures. Using suitable additives the grain sizes as well as the magnetic properties and the chemical composition of the grain boundaries can be tailored on the atomic scale leading to the desired properties.

Future development of new *multi-property* materials therefore requires interdisciplinary research activities, where the development of intrinsic properties as well as investigations of the microstructure and of local chemical compositions are carried out. The development of magnetic alloys is based on 27 elements of the periodic table leading to ~ 2100 binary and ternary ferromagnetic alloys from which only the binaries and a few ternaries have been investigated. Investigations on quaternaries or quinaries so far are restricted to FeSi- and SmCo-based systems. Insofar a wide field of opportunities is still open for new research projects.

In order to obtain *high-remanence* materials the dominance of Fe is a pre-requisite. High-coercivity materials either have to use rare earth metals in uniaxial crystals or transition metals as Co, Fe and Pt in strongly uniaxial crystals, e.g., CoPt, FePt. *High-permeability materials* require large spontaneous magnetization, vanishing magnetocrystalline anisotropy and vanishing magnetostriction. A further breakthrough for these materials could be achieved if nc alloys with a larger spontaneous magnetization; however, still a low magnetostriction could be found. The presently used Fe_3Si-based alloy, the so-called Finemet, has a spontaneous magnetization of 1.25 T. The use of a FeZrB alloy could raise J_S to a value of 1.5 T. Also the Curie temperature would be improved and could be further raised adding Co. The fine-shaded region in Fig. 2.14 shows the future possible improvement by using optimized nc-alloys.

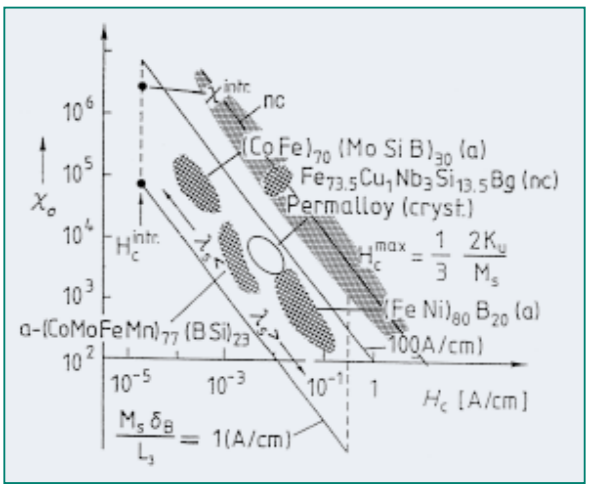

Fig. 2.14. Upper and lower bounds for χ_0 and H_c of soft magnetic materials based on the fundamental relation $\chi_0 \cdot H_c = M_s \delta_B / L_3$ (M_s = spontaneous magnetization, δ_B = domain wall width, L_3 = domain wall distance). Lower bound $M_s \delta_B / L_3 = 1$ A/cm. Upper bound 100 A/cm. The fine-shaded region indicates a future upper bound for nanocrystalline materials $M_s \delta_B / L_3 = 1000$ A/cm.

High-coercivity materials are based on the intermetallic compounds $Nd_2Fe_{14}B$, $SmCo_5$ and Sm_2Co_{17}. Deficiencies of these compounds are the low Curie temperature of

$Nd_2Fe_{14}B$ (T_C = 312°C) and the low spontaneous magnetization of $SmCo_5$ (1.05 T) and Sm_2Co_{17} (1.25 T). This allows applications only up to 100°C for the NdFeB systems and the maximum energy products of the SmCo systems are a factor of 2 – 3 smaller than that of NdFeB. Fig. 2.15 presents the development of the so-called maximum energy product $(BH)_{max}$ during the last century. This quantity is a measure of the energy stored by a magnet outside its volume. The shaded region shows the progress, which could be achieved if a FeCo-based magnet with a large spontaneous polarization of 2.45 Tesla could be realized by introducing strong planar pinning centres.

A breakthrough for the NdFeB type systems would be achieved for Curie temperatures of the order of 450°C because of possible applications in the car industry. In any case the use of NdFeB magnets for the electric energy production in wind mills will be a breakthrough concerning their efficiency and costs. Because of the smaller volumes of motors based on NdFeB magnets many new applications have become relevant, e.g., elevator motors or hybrid engines in car industry. However, higher Curie temperatures would even accelerate the acceptance of these magnets in the electro motor industry. In order to achieve this, far more additives have to be investigated in the NdFeB systems.

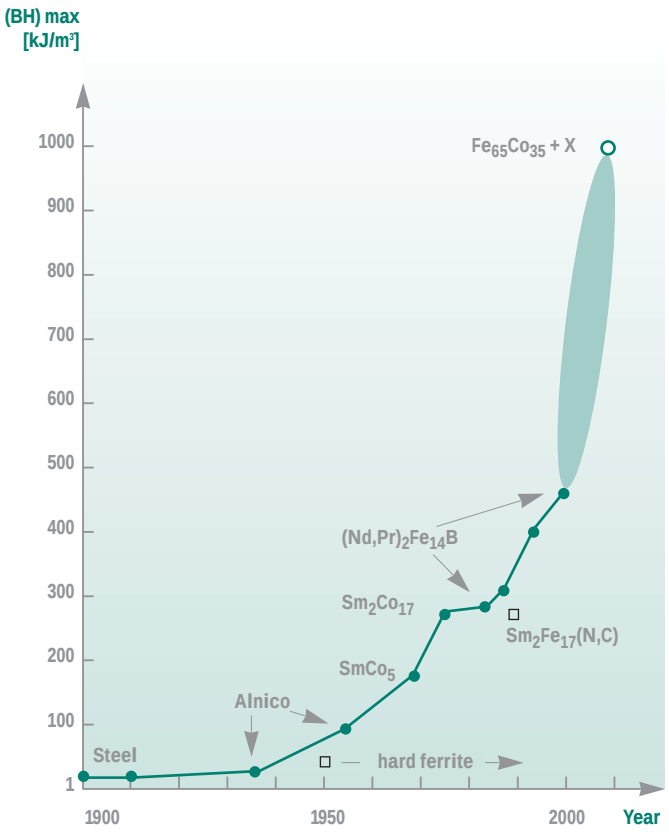

Fig. 2.15. Progress in improving $(BH)_{max}$ over the last century. The shaded region covers hypothetical FeCo-based alloys, which are magnetically hardened by additives X.

The production of *nc-composite hard magnetic materials* as, e.g., $Nd_2Fe_{14}B$ + α-Fe or $Pr_2Fe_{14}B$ + α-Fe would improve the situation of isotropic *bonded magnets*. Due to the large magnetic moment of α-Fe and the effect of exchange coupling maximum energy products of $(BH)_{max} \cong 100\ kJ/m^3$ could be achieved. These values are 40% larger than the values of conventional bonded magnets. In particular the application of small-sized powerful electromotors in audio and video devices as well as in computer peripherals results in an increasing demand of resin bonded RE magnets. The powders required for bonded magnets are manufactured either by rapid solidification techniques or by the so-called HDDR (Hydrogen Desorption Decomposition Recombination) process. The melt-spin technique produces isotropic magnets with large coercive fields with an enhanced remanence due to exchange coupling between the nanograins. The HDDR technique allows the production of aligned sintered magnets with large remanence. It is decided by the costs and type of application, which one of these techniques has to be used.

For technical applications of *giant-magnetostrictive materials* in micromechanical systems the Curie temperature (T_C ~ 100°C) of the amorphous FeTbDy alloys (Terfenol) is a serious drawback. A breakthrough would be achieved if the amorphous alloy could be nanocrystallized, i.e., achieving Curie temperatures of 320°C. The nc microstructure is a requirement in order to keep the coercive field small and to obtain a large permeability. Multilayered systems of FeTbDy/Nb may fulfil these conditions because the grain size is determined by the film thickness and the Nb-layer does not dissolve in the FeTbDy-layer. High magnetostrictive permeabilities are obtained by soft magnetic interlayers. Because of the interplane diffusion during nanocrystallization the magnetostrictive layer is destroyed. It is on open question how to avoid this deteriorating effect.

The *giant-magnetoresistance or GMR* is a prominent example of modern magnetism. The GMR in multilayers is due to the variation of the angle between the magnetization of consecutive magnetic layers, which are separated by a nonferromagnetic layer. Under certain conditions the coupling between neighbouring layers is antiferromagnetic producing a large electrical resistivity, which decreases drastically if an external field aligns the magnetization of all magnetic layers in parallel. The antiparallel alignment in zero magnetic field is a consequence of the interlayer exchange coupling. The GMR effect also has been observed in spin-valve structures, multilayered

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nanowires and granular systems. The GMR effect is used in devices such as sensors, read heads and nonvolatile magnetic random access memories (MRAMS). The GMR research furthermore revealed a new class of magneto-transport phenomena obtained in nanostructures by employing the spin polarization of carriers. Examples of this field of spin electronics include spin injection, spin dependent tunnelling and magneto-Coulomb blockade.

Giant-magnetoresistive thin film systems require a high time stability and well-defined switching times for magnetization processes. This can only be guaranteed by a reproducible microstructure, e.g., well-defined interlayer boundaries. The existence of statistically distributed nucleation centres at film boundaries or at edges leads to large spectra of coercive fields and a tremendous increase in noise of magnetic read signals. Accordingly, the production of perfect highly homogeneous multilayer systems would be a breakthrough in this field. The GMR devices then may be used as nonvolatile MRAMS, marking the first successful joint venture of magnetic materials and silicon technology.

A breakthrough in the *colossal magnetoresistive (CMR) systems* of manganites requires high-permeability materials, i.e., the so far available ceramic materials should be replaced by large grain or single crystalline materials in order to reduce the coercive field down to the 1 mT range. This means new preparation techniques have to be applied to make these systems useful for magnetosensoric, spin-induced tunnelling and pressure sensors. Here the tailoring of the microstructure is the dominant task to be solved. There are considerable fundamental and technological interests concerning the electronic correlation effects in the CMR systems. Double exchange, superexchange and dynamical Jahn-Teller distortions, charge and orbital ordering have to be investigated. Furthermore, the application of manganite perovskite films in hybrid systems with semiconductors where spin injection proceeds into the semiconductor deserves further exploration.
Molecular magnets suggest a wide field of applications in nearly all technological fields reaching from conventional electrotechniques as microwave technique to medical applications, the sensor technology and the recording industry. A breakthrough is expected if the Curie temperature of these materials can be raised above 100°C. This may be achieved by coupling of the ferromagnetic molecules by another intermolecular magnetic ion.
Self-organized superlattices either produced by ferromagnetic particles or wires of FePt or CoPt or by a *nanostructurized substrate* may be a future recording medium for the Terrabit/inch^2 recording density. A breakthrough is expected if these superlattices can be produced perfectly in scales of inches.

2.7.4. Research Directions/Priorities During the Next Decade

Further development of magnetic materials requires extended studies of phase diagrams of multicomponent systems and the magnetic, electrical, structural and chemical characterization of grain boundaries and intergranular phases. Future research activities should put the following priorities:

1. Development of nc-magnets with large Curie temperatures, $T_C > 400$°C, and large spontaneous magnetization, $M_S > 1.6$ MA/m, for all kinds of applications (high-permeability, high-coercivity - giant magnetostrictive materials). Energy products of ~ 1 MJ/m^3 for permanent magnets and energy losses < 100 kW/m^3 for soft magnetic materials at high frequencies of MHz.

2. Differential analysis of phase diagrams and of the microstructure on atomic scales with respect to magnetic properties, constitution and chemical composition of grain boundaries. Combined application of several experimental techniques (EDX, EELS, TEM, AFM, STM) and of computational solid state physics.

3. Characterization of magnetization processes in the nanometre range by advanced magnetooptical techniques (magnetooptical Kerr effect, Circular dichroism, Lorentz microscopy) as well as atomic force and tunnelling microscopy.

4. Developing materials for magnetocaloric refrigeration.

5. Developing semiconducting magnetic materials for spintronix combining the silicon technology with magnetism.

6. Development of large-scale superlattices of self-organized ferromagnetic nanoparticles or nanowires in patterned substrates for high-density nonvolatile recording in the range of Tbit/inch^2.

7. High-coercive thin film multilayers for high-density magnetic recording. Study of induced perpendicular anisotropy.

8. Computational micromagnetism for the determination of magnetic ground states and the dynamics of magnetization processes in small particles and thin platelets.

The efforts to achieve these goals should not be underestimated. Systematic, semi-automatic methods of combinatorial materials science are now being enlisted in the search for new ternary and quaternary phases. Computational

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electron theoretical methods have been developed to the point where intrinsic magnetic properties of new phases can be predicted. At present magnetic moments of intermetallic compounds can be estimated by means of the local density approximation and there is progress towards accurate estimates of the anisotropy energy and Curie temperature. The history of magnetic recording shows how a dominant technology produces continuous improvement year by year. Magnetic storage densities have been increasing at a rate of 60 - 100% per annum over the past 20 years and have now arrived at Gbit/cm^2. The maximum energy product of permanent magnets doubled every twelve years throughout the 20th century.

Just recently the development of nanosized systems including thin films and multilayered systems has led to new phenomena and novel applications. Further developments in these areas, combined with fundamental studies, will continue to have a strong impact on technology. It is evident that any materials breakthroughs are expected in nano- and thin film technology. Further progress requires considerable expertise and also a multidisciplinary approach. Naturally, there are clearly-understood physical limits to future progress; the superparamagnetic limit in small particles; the ultimate maximum energy product $(BH)_{max}$ is limited by the spontaneous magnetization of ferromagnetic materials.

2.7.5. U.S. – Japan – EU Positions

Activities on magnetic materials exist in all three countries. Also China and Korea have to be considered as strong competitors in magnetic materials. Singapore in future also will play some role. The handicap within the EU is the lack of an efficient recording industry. In so far the research on recording materials and systems is somewhat isolated. The required interaction between industry and basic research institutes cannot be initiated. In contrast these interactions exist in the U.S. and Japan being supported by the National Science Foundation, the NASA, the NATO (dominated by U.S.) and the MITI, respectively. Recent cooperations between Infineon and IBM will not improve the situation in the E.U. significantly because the BMBF may reduce the support for magnetoelectronics.

The situation is much better in the field of sensor techniques where the EU states have a worldwide leading position. Similarly in the fields of high-permeability and high-coercive magnetic materials the EU is able to compete with U.S. and Japan. In particular the EU magnet industry has to be considered as the leading one concerning the high-quality soft and hard magnetic materials. Concerning the research and development of new materials in U.S. as well as in Japan there exist considerable efforts to develop new magnetic materials with optimized property-spectra.

In U.S. as well as in Japan it becomes more and more usual to involve several institutions with supplementary know-how for the development of new materials. This has been recently demonstrated by NATO conferences entitled “Magnetic Storage Systems Beyond 2000” and “Magnetic Materials for Power Applications”.

At different laboratories in EU exist the experimental and theoretical background for the development of materials with wide property spectra. In particular the basic knowledge on fundamental physical, chemical and microstructural properties is available, i.e., the interdisciplinary collaboration could be successfully performed between the different departments.

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2.8. Superconducting Materials

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2.8.1. Introduction

Science and technology of superconductors have strongly progressed in the last years, and the development has reached an industrial level, for classical (metallic) as well as for High Temperature Superconductors (HTS). The compounds Y(123) and Bi(2223) (see Table 2.2) have clear commercial potential and are the focus of strong parallel academic and industrial research efforts worldwide.

Compound		T_c (K)
$YBa_2Cu_3O_7$	Y(123)	93
$Bi_2Sr_2CaCu_2O_8$	Bi(2212)	92
$Bi_2Sr_2Ca_2Cu_3O_{10}$	Bi(2223)	110
$TlBa_2Ca_2Cu_3O_{10}$	Tl(1223)	122
$HgBa_2Ca_2Cu_3O_{10}$	Hg(1223)	133

Table 2.2. Promising HTS compounds.

Future superconductor applications include advanced preparation and characterization technologies, down to the nanometre scale. Possible use of HTS materials can be subdivided in two main areas:

- Large scale *energy-related* applications (generation, transport, transformation and storage of electrical power), and
- Small-scale *electronics-related* applications (passive and active signal processing).

Over the last years, large size demonstration prototypes (transformers, power cables, current limiters, magnets, etc.) have been fabricated and successfully tested. Applications as current leads for low temperature systems, magnets and filters for mobile telephone base stations, have already made it to the market. Solenoids for MRI applications are an upcoming future market.

In many cases, the technical performance of superconductor applications is already superior to that of classical technologies, but production and material costs are still too high for economic competitiveness. Strong efforts in materials research, both at the laboratory and at the industrial scale, have to be done, but the *critical current densities*, j_C, in HTS compounds are inherently very high (>5 x 10^6 A/cm^2), in order that these materials will become economical, either in a mean or a long term.

2.8.2. State of the Art

Several projects related to HTS materials have been supported within the 5th Frame Programme. The research 2000/2001 in applied superconductivity covers four categories:

(a) Basic research: mechanisms of superconductivity and new superconductors

Basic research in HTS has focused on three main topics:

- The origin of superconductivity in these compounds. The actual mechanisms leading to superconductivity are still controversial. It has been predicted from optical measurements of the energy gap that the maximum *superconducting critical temperature* (T_C) for cuprates containing CuO_2 planes may be about 180 K. If the causes for the actual limitation could be understood, T_C of cuprates could be substantially increased. It is not excluded that new material classes with high T_C values will be found, an example being the recently discovered compound MgB_2 with T_C = 39 K.
- The processes limiting the current transport. While T_C for a given HTS compound does not much vary from one sample to another, the values of *critical current density*, j_C, and *irreversibility field*, B_{irr}, are extremely sensitive to changes, depending on synthesis techniques. When optimizing j_C at 77 K and appreciable magnetic fields, it is essential to introduce strong flux pinning centres dispersed in sufficient concentration. Chemical substitutions in HTS have had positive effects on $B_{irr}(T)$ and j_C.
- The phase relations involved in the synthesis of these ceramic materials. Precise knowledge of these phase fields is indispensable if one wants to improve the superconducting properties of HTS.

(b) Energy applications: tapes and wires

Superconducting energy applications such as *power cables, transformers and fault current limiters*, require the availability of thermally and mechanically stable, long conductors. The j_C values of industrial Bi(2223) *multifilamentary tapes* with a high degree of texturing are shown in Fig. 2.16, left.

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A second material class is now being considered as a serious substitute for Bi-based compounds: Y(123) *coated conductors*, where the biaxially textured superconductor is coated on a flexible metal ribbon. These conductors exhibit excellent properties, j_C less affected by the presence of appreciable magnetic fields, as shown in Fig. 2.16, right. The corresponding deposition techniques (see Sect. 2.8.2.(d)) for long lengths (>100 m) are still under development, while conductor lengths of >2 m with j_C values close to 10^6 A/cm^2 have already been prepared. Future research will focus on cheaper deposition methods, which may vary depending on the envisaged particular application.

Bulk melt-textured HTS materials allow novel applications, e.g. magnetic bearings and magnetic shields. Flywheels demonstrators have already been produced on a trial basis. Bulk superconducting materials for rotating machines with high current load require j_C values as large as possible.

Regardless of the chosen superconducting material, j_C increases with higher crystal defect concentrations, obtained by high temperature plastic deformation, nanoparticle doping, chemical doping or irradiation. *Examples:* In Y(123), enhanced flux pinning has been obtained by rare earth (R.E.) substitutions on the Y site. The addition of Ca to Y(123) has shown to have a beneficial effect on the pinning at large angle grain boundaries. Both results have been obtained in European laboratories.

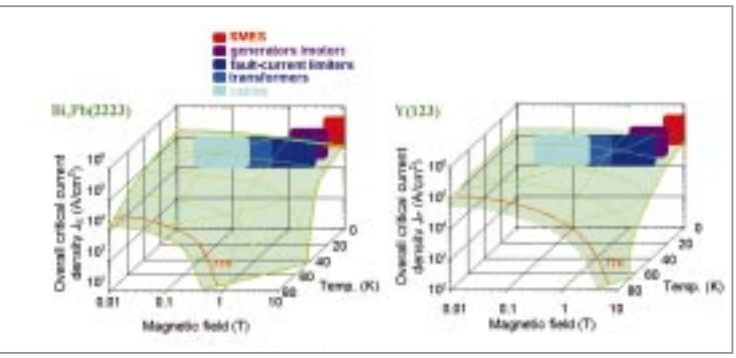

Fig. 2.16. Overall critical current density of state-of-the-art conductors, Bi(2223) (left) and Y(123) (right), as a function of magnetic field and temperature. The filled areas on the back-plane delineate the approximate field and current requirements for various applications.

(c) HTS electronics

Passive HTS devices such as filters with excellent quality factors have already made it to the marketplace. The outstanding challenge for HTS is to develop a fabrication route that will result in reliable and reproducible junctions for active device applications such as rapid-single-flux-quantum (RSFQ) logic circuits or SQUID magnetometers. VLSI technology is already in use for low temperature superconductor (LTS) (Nb/Al/O/Al/Nb) junctions, with operational devices with > 10000 Josephson devices per single chip already achieved. Most electronic and microwave device structures are based on thin films grown on appropriate substrates: LTS Nb-based technology is already well developed, that of NbN slightly less. This is in contrast to HTS films, which need to be grown epitaxially on single crystal substrates; but their superconducting properties are close to the intrinsic limit values.

(d) Film deposition techniques

Several deposition techniques have been developed for fabricating HTS films. For each HTS compound, the deposition route has to be optimized individually for satisfying the prerequisites for commercial use of film-based applications. It appears that only the full control of deposition techniques, allowing high j_C values in *layers considerably thicker than 1* µm will lead to a larger success of superconductors. So far, all known deposition techniques allow to reach j_C values above 5 x 10^5 A/cm^2 at 77K, 0T, for thickness still below 1 µm. There are various deposition techniques:

Laser ablation and pulsed laser deposition, which are widely used in research laboratories, are powerful tools for synthesis and preliminary investigations of new phases. The required small targets can be prepared in many laboratories, and stoichiometry is retained from the target to the film. This method can be applied for the fabrication of long tapes.

Ion Beam Sputtering and Thermal Coevaporation (also on *Inclined Substrates*) are particularly suited and cheap for uniform films over large areas. The former appears to be also promising for scaling-up the film production. A European team has deposited YBCO films using coevaporation technique on substrates as large as 20x20cm^2 and reported jc values of ≤ 2x10^6 A/cm^2.

Magnetron sputtering and Molecular Beam Epitaxy have been shown to produce high-quality films: these techniques appear to be suited mainly for thin films and/or investigation of new hybrid structures, multilayers and devices. Special attention must be paid to growth by Liquid Phase Epitaxy.

Chemical non-vacuum techniques: Very high j_C values, >3 x 10^6 A/cm^2 have been obtained on Y(123) layers by using *metal organic deposition* and MOCVD. Very recently, high j_C values were also obtained for Spray Pyrolysis, a relatively simple technique with high technical promise.

A limitation is common to all these techniques: j_C decreases for film thickness ≥ 1 µm, thus lowering the total *critical current*, I_C, probably due to local stresses: Strong progress is needed.

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2.8.3. Future Research Visions and Expected Breakthroughs

Future R&D will aim towards higher j_C values, improved yield and lower material consumption, in order to bring the manufacturing price down to a competitive level. However, *further breakthroughs* can only be achieved by means of strongly increased effort in basic research in academic laboratories.

(a) Basic research

Future *basic materials research* must contain a strong effort towards the synthesis of some very high T_C materials. *New synthesis methods* have to be found, replacing the actual laboratory methods (e.g. high pressure synthesis, at > 5 GPa) by industrial techniques. Further efforts are also needed with respect to *current limiting mechanisms* in HTS and possible materials-related solutions. Although it is well established that both grain boundaries and flux line dynamics are two important limiting factors, the materials science needed to tackle these issues on a nanometre scale is still far from complete. Goals are:

- Optimization of T_C, j_C, and H_{irr} in HTS superconducting systems exhibiting small anisotropy.
- Reduction of toxic element content in Tl(1223) and Hg(1223), by substitutions.
- Further studies of the mechanisms in HTS materials, in view of higher T_C in existing systems.

(b) Energy applications

i) Bi(2223) tapes Actually, industrial Bi(2223) tapes in km length can be produced, with j_C values above 35 kA/cm^2, e.g. engineering je values > 20 kA/cm^2. However, these values should at least be doubled to be economical: a substantial change of the industrial fabrication methods is needed. Goals are:

- Calculations and experiments on details of the high temperature phase diagram.
- New reaction paths for tapes with core density ≥ 80% and improved formation kinetics.
- Fabrication of *round* Bi(2223) wires with high j_C values and low losses in ac regimes.

ii) Y(123) coated conductors Y(123) may be the superconductor for the next decade, due to higher field tolerance, but also due to expected lower production costs with respect to Bi(2223). The actual thin film material is excellent, but on small scale processes only. Goals are:

- Coatings of thickness well above 1 µm without decrease of j_C.
- Improvement of chemical (non-vacuum) deposition techniques.
- New characterization of deposition parameters for improving the process reproducibility.
- Scale-up of tape production to lengths > 100 m, e.g. for cables, magnets, energy storage, etc.
- Scale-up of targets to diameters > 200 mm, e.g. for current limiters, etc.
- Further development of known alternative materials with higher T_C: Tl(1223), Hg(1223), etc.

iii) Melt-textured bulk HTS The development of the processing techniques for bulk HTS of complex shape and composite components and with very low resistivity is essential. The relevant properties for these materials are the current densities, the magnetic fields, their distributions, the levitation force, the losses, and the mechanical and thermal properties. Goals are:

- Processing techniques for complex shapes with very low resistivity, e.g. flywheels, etc.

(c) HTS electronics

Less expensive processing routes and cheaper buffered substrates are needed, if a really broad mass market is to be exploited. Many circuits will incorporate other materials, e.g. ferroelectrics, ferrites or colossal magnetoresistive materials. Completely new technologies may have to be developed to achieve the necessary reproducibility for HTS junctions. This will require new material engineering for understanding the limiting factors for the performance of junctions and for providing the necessary characterization tools. Europe should consider supporting one or more central foundries for the fabrication of thin films and devices, with a micron or less lithography. The first foundry could be devoted exclusively to the LTS materials. A programme should also be initiated in HTS thin films and junctions for any kinds of applications, including *medical applications*. Major collaborative programmes are needed for improving understanding and performance of HTS films for microwave applications and of junctions for SQUID and RSFQ applications. A major development programme is also needed on large area thin film processing for faster and less expensive film deposition, as a vital component of future “wireless communication systems”. Note that the last point is also valid for the coated conductors mentioned above. Goals are:

- Improvement of performance of thin films and substrates
- Scale-up to large area processing and reduction of the costs of thin films and substrates
- R&D for reproducible multilayer technology for integrated junction circuits and for dielectric substrates for microwave films
- Central foundries for the fabrication of LTS devices with lithography at submicron range.

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2.8.4. Comparison with U.S. and Japan

A strong competition exists between the laboratories and industries in the EU and those in U.S. and Japan. Each region has different centres of gravity, but that similar trends can be observed:

- *Bi(2223) tapes:* Bi(2223) multifilamentary tapes are actually the only product being already on the market, in U.S. (market leader), EU and Japan. This conductor is still far from being optimized: new efforts have started, in several laboratories and industries of EU, and Japan.
- Y*(123) coated conductors:* For certain applications, Y(123) coated conductors are superior to Bi(2223) tapes (higher field tolerance, expected lower production costs). In this field, European laboratories (in collaboration with industries) have thus developed a strong activity, and their level is at least equivalent to that in U.S. and in Japan.
- *HTS electronics:* The industrial engagement is much higher in U.S. and Japan, which explains that the volume of this activity in the EU is somewhat smaller. However, this subject should be highly funded, also due to the implication of miniaturized devices in promising future applications, in telecommunication, but also in medical applications.

2.8.5. Conclusions

Breakthroughs in the field of superconductivity are intimately related to the progress in material research. The fundamental aspect of material research, and in particular also the search for new approaches, must be intensified in order to maintain the contact with U.S. and Japan in this field. Developments in the field of applied superconductivity imply a great variety of material aspects, reaching from the study of bulk materials to the development of long conductors with filaments (or coatings) of sizes down to ≤ 1 µm. The fabrication of devices (used in many fields, including medical applications) requires the technology for local material control at a scale of a few nanometres.

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2.9. Materials for Fusion

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2.9.1. Introduction

Materials issues are of vital concern for the development of fusion energy into a sustainable source of energy supply. Advances in plasma physics and thus in fusion device performance have been flanked by an increasing understanding of the environment to which materials are exposed in fusion devices and by the development and application of new materials. In Fig. 2.17 the progress of the plasma performance is shown as triple product of plasma density, plasma temperature and energy confinement time. These data are related to the introduction of new materials for plasma facing applications. The Q=1 line indicates the break-even condition at which fusion power output equals the external power input into the plasma. Near-break-even conditions in present fusion devices (JET, JT-60U) have been reached with the help of surface and materials sciences. Now the emphasis is on power-producing fusion systems and the related materials research.

In this respect, the next step in the world-wide fusion programme, ITER [1], Fig. 2.18, has to be the main aim allowing the calibration of operational requirements with materials performance in terms of chemical, thermophysical and thermomechanical properties. At the same time materials development for fusion has to be pursued aggressively. On one hand an intense neutron source has to be built and operated to qualify base line materials for fusion reactor applications. On the other hand intense basic research into new materials is needed to offer fusion as an attractive and competitive energy system to society.

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2.9.2. State of the Art of Materials Research for Fusion Technology

The requirements and thus also the materials themselves depend strongly on the specific application in a fusion reactor, Fig. 2.18. Here, a distinction is made between "structural material", "breeding material" (not being treated in this article), "plasma facing material", and other materials for special applications.

(a) Structural materials

In most exposed locations the structural materials of a fusion reactor would be subjected to neutron-induced atomic displacements of up to 30 dpa (displacements per atom) per operational year. This is accompanied by volumetric heat deposition and by the strongly material dependent bulk production of gas atoms (especially H, He).

The baseline development covers ferritic-martensitic steels with tailored elemental composition for reduced neutron activation. The latest development is the EUROFER alloy in which elements with high cross sections for activation by fusion neutrons have been substituted by more benign elements, e.g. Mo has been replaced by W; Nb by Ta and V. The Cr content has been adjusted to optimize corrosion resistance and low embrittlement under neutron irradiation. The long standing research and development in this field resulted in a material which is expected to withstand neutron fluxes up to 150 dpa and which allows an operational temperature range of 300°C to 560°C. Thus a structural material would be at hand to build DEMO, a power-producing demonstration reactor after ITER [2].

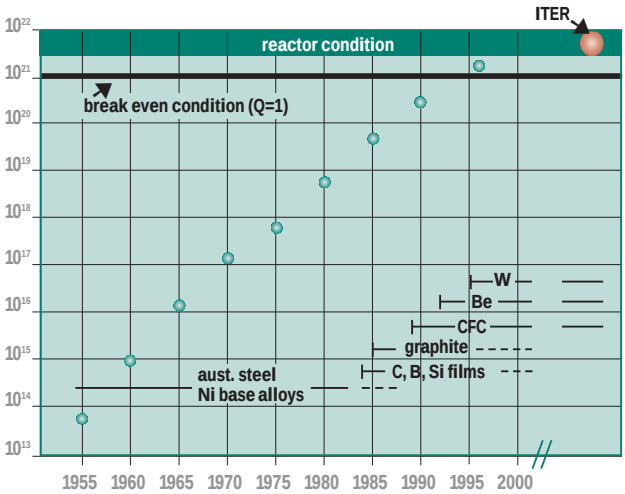

Fig. 2.17. Progress of the fusion triple product of plasma density, temperature and energy confinement time ($nT\tau$) Q=1 means fusion power output equals external energy input. The field "reactor condition" marks the operational field of fusion reactors. ITER is the international next step in fusion development. The plasma facing materials applied for high heat flux components are indicated.

Exploratory work is being performed on dispersion-strengthened steels, which would allow for operation at higher temperatures.

Materials, which are extremely attractive in terms of their low activation under neutron irradiation, are vanadium alloys and ceramic composites (SiC-SiC). Current knowledge hints that for these materials intense basic research is needed to allow for the application in fusion.

(b) Plasma-facing materials

Of the total fusion power in a reactor at least 20% will be deposited on the surface of the plasma-facing components. The divertor surface will see local heat loads of the order of 10 MW/m^2. Transient heat loads in present devices can be much higher, but intense research effort in plasma physics is being invested into the development of control mechanisms against such operational transients.

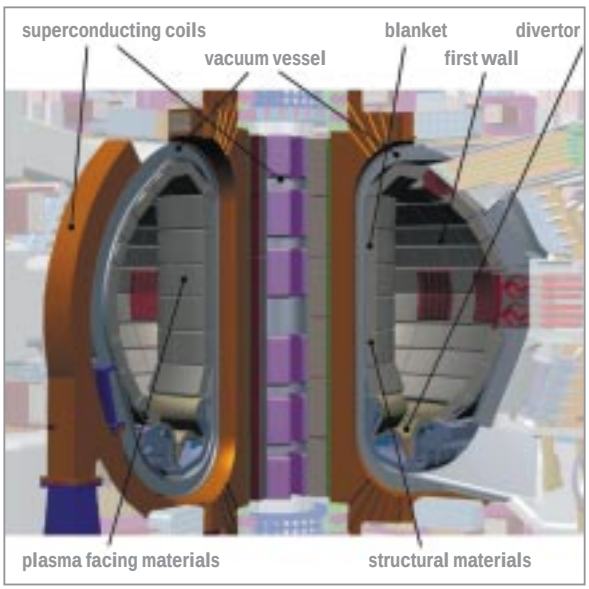

Fig. 2.18. Main components and materials for ITER.

Components and materials for plasma-facing applications have seen very fast progress during the last years. The growing understanding of plasma-material interaction processes has allowed the choice of applicable materials to be widened and has resulted in the selection of Be for the first wall, carbon fibre reinforced carbon (C/C) composites and W for the divertor of ITER [3]. Recent milestones in the field were

- understanding of transport processes and materials migration in fusion devices ("erosion and redeposition"),
- successful use of low Z composite materials and films during the operation of near Q=1 plasmas,
- development of dissimilar material bonds to remove steady state surface heat fluxes up to 30 MW/m^2.

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In addition to these major activities in structural and plasma-facing materials advances were made with special materials for critical applications, e.g. the use of 10 cm diameter diamond windows for 1 MW microwave power transmission.

Finally, it has been shown that materials for the superconducting coils are mature and ready for reactor grade application.

Europe and Japan are presently leading the field of fusion materials science. U.S. efforts have severely suffered as funding for fusion research has been cut, because the need for a long term supply of sustainable energy is not being regarded as a high priority within the U.S.

Japan has a wealth of research activities in this field with mainstream development of fusion materials being carried out by a national research institute (JAERI) and strong basic research in the field of radiation effects and material studies being carried out by universities. Subjects include low activation steels, vanadium alloy development on industrial scale, and pace making work on advanced SiC/SiC composites

In Europe the member states of the EURATOM programme perform co-ordinated research in the fusion materials field with participation from mostly non-university institutions. The materials programme, which is being carried out under the European Fusion Development Agreement (EFDA), mainly supports application-oriented research. Most of the effort is dedicated to low activation steels, exploratory work being done on dispersion strengthened steel and other alloys as well as SiC/SiC composites.

2.9.3. Expectations and Needs for the Next ten/twenty Years

ITER will be the centre piece of the European fusion programme. Regarding materials issues, during operation of ITER the boundary conditions for the use of materials in a reactor relevant environment will become precisely known. Plasma-material interaction processes should be understood and the heat flux removal technology should become mature.

The steady development of structural materials, especially of steels with low activation properties should result in a qualified material for building a first generation power reactor. For this and for the testing and qualification of any other fusion reactor material a 14 MeV neutron source is definitely needed. This facility will provide a neutron environment very similar to that in a fusion reactor, however the local neutron flux density will be higher and thus allow accelerated irradiation. The planning of this "International Fusion Materials Irradiation Facility", IFMIF is being carried out internationally under an agreement of the International Energy Agency, IEA. Expected costs to be shared internationally are 600 M€ [2].

In parallel to this evolutionary process of materials development and qualification, basic research in the field of materials science is urgently needed. Here the aim is towards a breakthrough in new materials with which fusion can be offered to society as a highly attractive and competitive energy system. Regarding such new materials the most important questions are:

(a) To which performance can advanced low activation materials be developed?

Directions are to increase the operation temperature for optimum energy conversion efficiency and to further improve the low activation properties of the materials. Possible paths are oxide dispersion strengthened steels, metal matrix – ceramic fibre composites, SiC/SiC composites, and possibly vanadium base alloys [3-5], Fig. 2.19.

Break through and success in this field would permit the highly loaded components in a fusion reactor to be furnished with materials having high strength also at temperatures well above 560°C (900°C in the case of SiC/SiC) and having highly favourable low activation properties. This would allow the thermal efficiency of a fusion power plant to be increased well towards the 50% mark. The behaviour under neutron irradiation is critical with such complex advanced

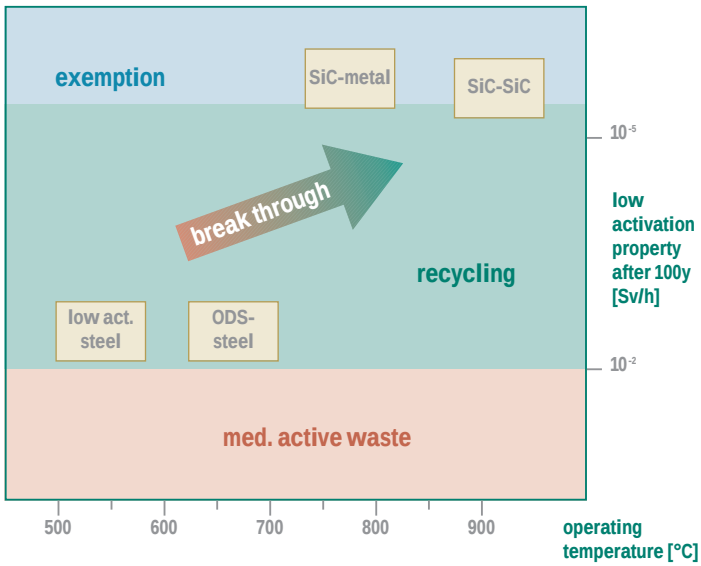

Fig. 2.19. Aiming at a breakthrough in structural materials. High temperature materials, which can be easily recycled or exempted after reasonable time, will underpin the attractiveness of fusion as an energy system.

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materials and needs to be understood from the atomic scale to the mechanical property level of the materials.

(b) To which degree can thin films reduce the tritium uptake of structural materials?

The tritium uptake of the structural materials and the migration into the coolant should be reduced as far as possible in a fusion reactor in order to minimize the tritium quantity, which could be accidentally released.

The advances in atomic thin film deposition by plasma-assisted methods and the possibility to tailor the nanostructure of these films during deposition open a new horizon in the development of permeation barrier coatings. Together with an evolving understanding of the atomic interface and the migration physics, a new generation of tailored barrier materials could be developed.

(c) Can plasma-facing materials with maximum lifetime be developed?

The use of high atomic number materials like tungsten would possibly allow to drastically increase the lifetime of the plasma facing components. However, the interaction of such materials with the plasma is extremely complex and needs to be controlled. If research in this field would be successful, the lifetime issue of the plasma facing material could be resolved. Work on ITER will show whether such plasma operation windows can be established, and perhaps even enable medium Z materials to be used. The thermal gradients in the plasma facing components, which are exposed to a surface heat flux of the order of 10 MW/m^2, will require advanced reinforced composite materials [6,7].

A further subject of intense research concerns the joining technology of the plasma facing material to the heat sink, such that the high heat flux from the plasma can be removed.

In order to proceed along this path, the following *key* technologies are essential and have to be strengthened:

- Advanced metallurgy (e.g. compositionally tailored alloys; metal matrix composites) and joining technologies.
- High temperature ceramic composite processing (e.g. SiC/SiC).
- Thin film technology (e.g. permeation barrier coatings).

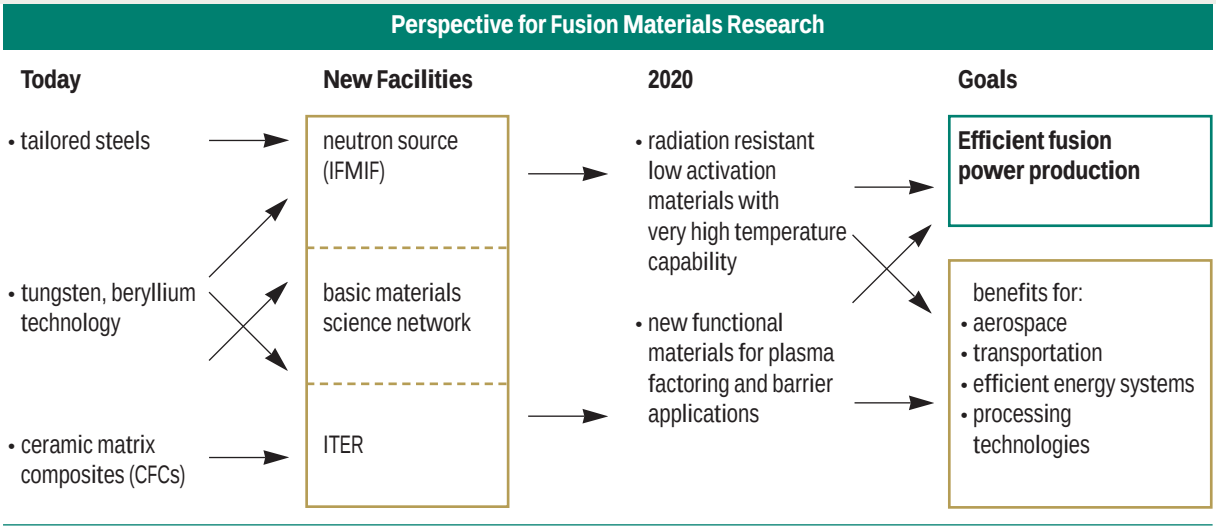

Fig. 2.20. Perspective of fusion materials research.

It is obvious that these three fields also are closely related to other advanced materials applications and that the results of this research will be highly valuable to other sectors, e.g. fuel cell and hydrogen technology (hydrogen permeation barriers); aerospace and transport technology (composites); plasma technology (advanced materials processing), Fig. 2.20.

2.9.4. Actions Proposed

A new initiative on basic materials science issues related to fusion is strongly needed and would be excellently placed within a EC materials science programme. It would directly enhance the performance of the EURATOM programme for the development of fusion energy.

Important actions within the EC materials science programme should be:

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- New alloys and composite materials for high temperature applications.
- Thin film processing - ceramic films with barrier functions.
- Understanding and control of radiation effects in complex materials.
- Facilitating the construction and exploitation of an intense neutron irradiation facility (IFMIF).

Integrating the competence of research laboratories (e.g. from fusion, aerospace, materials science), universities and industry into a "*network of excellence*" for the basic science issues of fusion materials would be the most appropriate step towards the aim of attractive and commercially viable fusion energy.

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2.10. Materials for Transportation

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2.10.1. Introduction

Rising energy prices and heightened environmental concerns are intensifying the global push for quantum gains in materials performance. In all major industries, there is an acceleration of the longstanding unfulfilled demand for lighter, stronger, and more affordable materials. The lack of a leap forward in materials performance continues to be a brake to progress in many industries, but no industry is constrained more by the long absence of a breakthrough in materials performance than the transportation industry.

Other industries have been spurred by breakthroughs and are making rapid progress towards goals once considered to be at the outer limits of their technological potential. For example, the Internet has revolutionized the telecommunications industry, and the emerging map of the human genome promises extraordinary progress in medicine and biotechnology. But, the materials industry has not achieved a comparable breakthrough. No outsized gains have been made in materials engineering in the past 50 years, and a revolution in transportation remains an apparition.

As a consequence, the transportation industry is increasingly reliant on composite materials. But, composites lack precision in their makeup and sufficient predictability in their performance, and their greater costs exceed their margins of performance versus traditional materials. As an alternative, materials scientists have explored foam technologies. But, like composites, foams lack precision and predictability, and the costly processes for producing foams fail to realize a balance between density and porosity. Thus, the long-awaited breakthrough in material performance remains elusive.

State-of-the-Art Materials in Transportation

Steel	Glass-fibre reinforced polymers
High strength steel	Graphite-fibre reinforced polymers
Aluminium	Polymeric composites
Plastics	Metal-matrix composites
Ceramics	Polymer-matrix composites
Magnesium	Ceramic-matrix composites
Titanium alloys	Structural composites
Advanced aluminium alloys	Intermetallics
Nickel alloys	Super alloys
Single-crystal nickel-base alloys	Microtextured materials
Aluminium lithium alloys	Self reinforcing liquid crystals
High temperature resin	Carbon-reinforced thermoplastics
Polyimides	Liquid crystalline thermosets

Fig. 2.21. In an effort to make products lighter, stronger, and more affordable, the transportation industry is relying on a wide range of increasingly more complex, scarce, and expensive materials.

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2.10.2. State of the Art of Materials Research in the Transportation Industry

To achieve extraordinary advances, the transportation industry requires materials that are lighter, stronger, safer, and more affordable than conventional materials (Fig. 2.21). Engineers are pursuing these ideal parameters through increased precision in both design and manufacture to achieve greater uniformity and concomitant predictability in materials performance. For example, engineers are developing nanoscale and microscale material systems, using computational combinatorial methods to develop new materials with novel properties, and integrating sensors and actuators into structures to make them "intelligent" [1,2]. Graded material concepts are being used to improve material distribution in structures and, at the atomistic level, engineers are developing manufacturing systems that use probes in atomic force microscopes to assemble atoms into precise molecular arrays of materials [3,4].

But, a breakthrough remains remote. Conventional engineering techniques have not evolved to achieve sufficient precision and uniformity to generate a dramatic increase in materials performance. The goal seems clear, however. A quantum gain can be achieved through a solution that aligns material mass with enough precision to optimize material distribution in a product. Historically, this has been a recurring theme in materials engineering, whether the search has been for maximum density or maximum porosity in materials morphology. So, it seems that the elusive solution may be a structural technology that is based on a calculus that balances the variation between the two extremes.

With such a technology in hand, materials research and development (R&D) could be brought into sharp focus, ending the wide-ranging and unresolved search of recent decades. Near- and long-term R&D agendas could focus on the deployment of this technology to achieve the long-awaited breakthrough in materials performance. These agendas could establish a clear strategy and direction for materials R&D to drive a revolution in transportation that would reverberate through other industries and throughout the European economy. Technological history suggests that, given the overlong and relentless search for such a breakthrough technology, it must be on the horizon. Indeed, by virtually any standard, it is long overdue.

2.10.3. Reflexive Material Technology

The most promising technology on the near horizon appears to be Reflexive Materials Technology™ (RMT™) [5]. This novel structural technology has the elemental underpinnings and potential for ubiquity that distinguishes a breakthrough technology. RMT affords the design, engineering, and manufacture of optimal structures, because it minimizes the amount of materials required to form a product, while optimizing the structural integrity of the product. Unlike current technologies, RMT provides both the design precision and fabrication control to produce products made of the least amount of material(s) sufficient to assure reliable stress/strain management according to performance specifications. With RMT, the ideal parameters listed above finally can be realized through a systems approach to materials development that combines structural solutions with materials & process solutions (Fig. 2.22). Such an approach was recommended for cost-effective and competitive materials development by the transportation industry in a 1993 study conducted by the National Research Council's Committee on Materials for the 21st Century [6]. RMT provides the quantum leap in materials performance necessary to ignite the long-awaited revolution in the transportation industry.

RMT engineering optimizes materials performance by controlling the manner by which structures are permitted to address load and, consequently, to undergo strain. It is particularly advantageous for weight-limited applications where a high strength-to-density ratio, high stiffness, and affordability are important. RMT operates independent of scale and materials, with the same effect, whether at the molecular (nano-) level or at the human-made (macro-) structural level. These characteristics provide an excellent springboard for quantum gains in materials performance that could rival the impact of the Internet on the communications industry and the emerging map of the human genome on medicine. The breakthrough in materials performance enabled by RMT could drive extraordinary advances in transportation and other weight-sensitive industries.

RMT achieves design precision and fabrication control through *distributed porosity*™. To strike the essential balance between density and porosity, RMT inculcates discrete, symmetrically aligned pores into structures made with metals, polymers, ceramics, composites, and other materials. This is the *RMT Architecture*™. The interplay of the symmetrically aligned pores, or *voids*, within an RMT-engineered structure, steers and spreads the stress

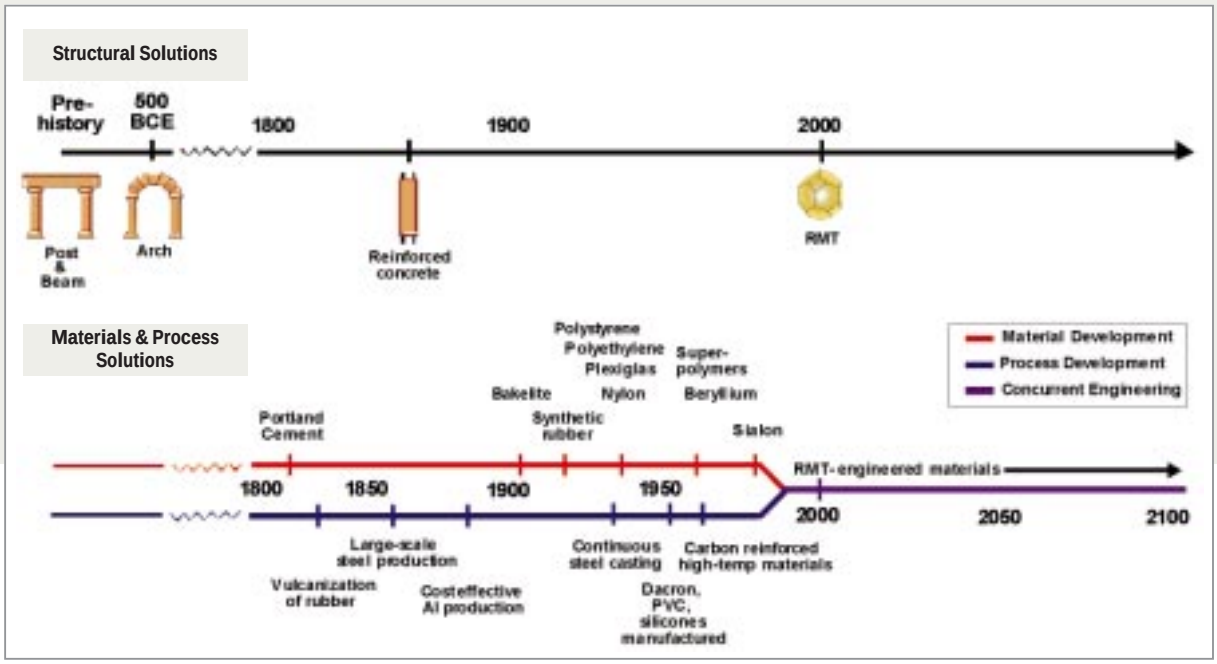

Fig. 2.22. Structural and materials & process solutions timelines.

of external loading along the truss-like struts of the RMT Architecture and throughout the structure. This *stress steering*™minimizes the development of tensile strain in a structure in favor of maximizing compressive strain.

The key to RMT stress/strain management is the sphere-like geometry of the Truncated Rhombic Dodecahedron (TRD), shown in Fig. 2.23. Figurative TRD cells shape an RMT structure, similar to the way soap bubbles shape a froth, or foam [7]. However, unlike the irregular distribution of bubbles in a froth, conjoined TRDs in RMT structures are aligned symmetrically in a face-centred cubic (FCC) configuration that spontaneously creates a corresponding FCC array of voids in the structure. The void array gives an RMT structure a framework, or skeleton, of the octa-tetra design. The struts of the *RMT Architecture* are triangulated and loaded axially and are short and fat to optimize their capacity to carry compressive load. This unique architecture generates an isotropic material response, producing the optimal mechanical response by RMT-engineered structures independent of the loading state. Each RMT-engineered structure is optimized for a particular application by a particular iteration of the *RMT Architecture*.

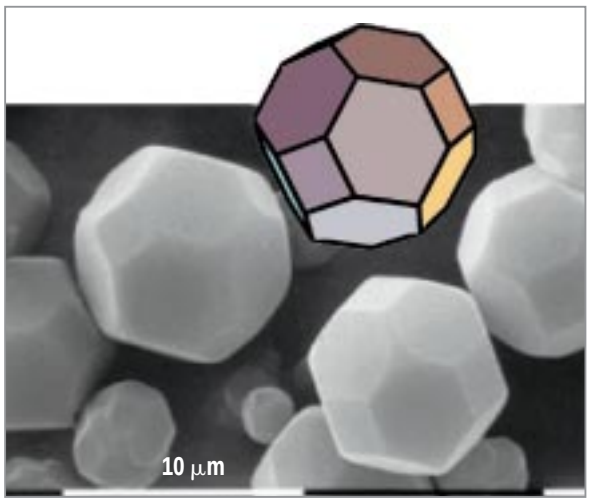

Fig. 2.23. Naturally occuring Truncated Rhombic Dodecahedron (TRD) in a mesoporous silica material [8] that might be the basis for self-assembling and self-healing RMT-engineered materials.

2.10.4. Computational Tool for RMT

To simplify and speed the design, engineering, and manufacture of RMT-engineered materials, products, and structures of uniform quality and performance, a new computational tool is required. Development of this computer-based tool must be a cornerstone of any near-term R&D agenda. The intent would be for this practical tool to permit the precision design, optimization, and manufacture of a vast number of RMT-engineered products with optimum ease and efficiency through computer-integrated manufacturing (CIM). The goal would be for this new enabling tool to allow engineers and others to use high-performance computing to inaugurate a

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new era in materials engineering and create a new generation of superior materials, products, and structures through RMT. The end-goal, of course, would be to afford the manufacture of commercial RMT-engineered products of uniform quality and performance at competitive costs utilizing CIM techniques. Developed specifically for RMT commercialization, *RMT rapid manufacturing systems*™ readily lend themselves to integration into CIM systems. RMT manufacturing systems are now in the patent process. Fortunately, it appears that through simple modification of conventional manufacturing technologies, *RMT rapid manufacturing systems* can be incorporated into most existing manufacturing facilities with only modest capital investments. Development of techniques for the rapid and cost-efficient integration of RMT manufacturing technologies into existing manufacturing plants and facilities would be integral to a near-term R&D agenda.

Near-term Materials R&D

- Computational tool for RMT design, engineering, and manufacturing.
- Retooling of existing plant and facilities for optimal utilization of RMT rapid manufacturing systems.
- Re-engineering of existing products.
- Optimal utilization of RMT rapid manufacturing systems to produce re-engineered products.
- RMT materials joining.
- RMT materials repair and recycling.

Fig. 2.24. Framed by RMT, industry priorities will dictate the agenda for near-term materials R&D to produce lighter, stronger, and more affordable products.

2.10.5. Near-Term Research & Development

While RMT can frame the agenda for near-term materials R&D, industry demands for lighter, stronger, safer, and more affordable materials must dictate near-term materials R&D priorities (Fig. 2.24). Thus, a prime near-term goal must be to re-engineer the architectures of existing products, components, and structures using RMT, to rapidly enhance the in-service performance of both intermediate and final products whose designs are already proven through practical application and use. The results promise to be extraordinary, because RMT requires at least 5% to easily 50% *less* material to make products and build structures that outperform today's versions. Simultaneously, near-term R&D must focus on the proper selection and optimal utilization of *RMT rapid manufacturing systems* for cost-effective production of RMT-engineered products and structures.

To rapidly achieve quantum gains in materials performance and ignite a revolution in transportation, near-term materials R&D must enable the development of RMT-engineered products and structures that yield significant economic, environmental, safety, and energy-related benefits. Near-term R&D must direct the efforts of transportation engineers, for example, toward exploitation of the advantages of RMT to achieve the optimal balance between performance and cost in existing vehicles, whether in the air, on the surface, or in the sea. Near-term utilization of RMT to re-engineer existing designs to create lighter, stronger, stiffer, and more affordable products would lead to:

- *Parts consolidation.* This will mean fewer welds, easier assembly, faster production rates, reduced labor and capital costs, and increased productivity.
- *Less framing.* RMT engineering will allow substantial reductions in framing to support the ubiquitous plates used to assemble vehicles, e.g., airplanes, tanks, cars, trains, and submarines. Increased strength and stiffness in RMT-engineered plates and panels will eliminate bowing or warping conventionally controlled by framing, lowering component and system costs.
- *Wider load distribution* in vehicles will increase durability. Each RMT-engineered part, component, and subassembly (e.g., an instrument panel) automatically will be load bearing, up to its material limit. Spreading load and eliminating concentrations of strain will reduce material requirements and enhance vehicle safety, performance, and durability.
- *Materials substitution* of less expensive materials in numerous applications will generate wide-ranging economic benefits, including direct and indirect cost savings.
  Improved fuel economy. Whatever the choice of materials in a vehicle, RMT engineering will make them lighter, whether the materials are iron, steel, aluminium, plastics, magnesium, ceramic, or other materials.
- *Reduced environment impact.* RMT-engineered savings in materials and fuels alone could have dramatic environmental benefits worldwide, including substantially reduced vehicle emissions.
- *Increased safety and reliability.* RMT-engineered improvements in toughness, durability, and reliability of parts and components will increase vehicle safety and consumer confidence.
- *Increased passenger comfort* by reducing interior noise, vibrations, and increasing handling and performance through sensor/actuators that track the environment and align the structure to optimize performance.

2.10.6. Long-Term Materials Research & Development

Long-term, R&D drivers are primarily economic, not scientific. Therefore, long-term RMT R&D must focus on the

development of new RMT-engineered products to satisfy the transportation industry's commercial agenda (Fig. 2.25). Historically, 95% of products that utilize a new technology are yet-to-be-determined at the inception of a technology's use. Long-term materials research must be aimed at developing affordable new materials, with economical and environmentally sound lifecycles (from raw material to repair and recycling), that can be produced in large quantities using "green" engineering concepts [6].

The focus must be to develop new materials that exploit the structural advantages of RMT, which emphasizes the compressive strengths of less expensive, less technical, and more abundant materials. New materials also should be developed to exploit the precision of *RMT rapid manufacturing technologies*, which emphasize low-cost, automated manufacturing processes that are continuous from raw material to finished product. Achieving long-term RMT materials R&D goals also must include continued refinement and development of computational tools to support a comprehensive concurrent RMT-engineering approach as part of evolving CIM technologies.

Long-term Materials R&D

- Develop new RMT-engineered products to satisfy the transportation industry's commercial agenda.
- Develop affordable new RMT materials with economical and environmentally sound lifecycles that can be produced in large quantities.
- Exploit structural advantages of RMT using less expensive, less technical, and more abundant materials.
- Develop new materials to exploit the precision of RMT low-cost, automated manufacturing processes that are continuous from raw material to finished product.
- Continue refinement and development of computational tools to support a comprehensive concurrent RMT-engineering approach as part of evolving CIM technologies.
- Develop educational programs to revive and replenish the ranks of materials and transportation engineers and scientists.

Fig. 2.25. Long-term materials R&D must satisfy the transportation industry's business agenda by exploiting the unprecedented commercial advantages of RMT.

While RMT is the long sought engineering solution that can trigger quantum gains in materials performance, it also is the solution for generating the verve and excitement that will restore youth to an aging industry. Reflecting a global trend, over the past seven years in the U.S. aerospace industry the number of workers ages 25-34 declined to only 17% of the workforce and the number of engineers and scientists performing R&D declined 30% between 1998-1999. Europe has a rare opportunity to exploit this trend to its competitive advantage by pioneering a technological breakthrough that will attract the energy and creativity of youth through open-ended opportunities for seminal innovations and the concomitant potential for extraordinary economic gains. To fully capture the advantages of RMT, Europe's long-term R&D agenda must include educational programs to replenish and revitalize its ranks of materials and transportation engineers and scientists.

RMT precision and predictability open a new era of concurrent innovation, allowing existing products to be improved and new products to be developed. To realize the promise of RMT, industry and governments must work in concert. Industry must be the prime mover and governments across Europe must provide critical R&D support and new infrastructure. In particular, industry and governments must combine and focus their resources via transnational and interregional cooperation to deploy a new generation of RMT-engineered transportation systems, including airplanes, ships, trains, and cars, along with the infrastructure to support these systems, including RMT-engineered runways, roadways, railways, bridges, and piers. These new transportation systems can be the foundation and impetus for an unprecedented and extended era of broad-based economic growth and prosperity in the European community.

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2.11. Materials Science in Space

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2.11.1. Introduction

Materials science in space is a small but challenging sector in the field of materials science. The environment of reduced gravity existing in space puts fundamental research in the field of materials processing within our reach. Under microgravity, the buoyancy convection in a melt is significantly reduced and sedimentation effects are suppressed. This enables the investigation of crystallization and solidification mechanisms with no interference from convective heat and mass transport in the liquid.
In this way, the reduced gravity level existing in space provides an important tool for fundamental research projects in materials science. Performing demanding experiments in a microgravity environment can therefore be regarded as a revolutionary approach in materials science.

2.11.2. State of the Art

Materials science experiments have been carried out in space for more than two decades. Solidification or crystallization processes are sensitive to melt flow or sedimentation effects. This implies that the experiments need at least some minutes of low gravity and therefore can only be carried out during sounding rocket flights, during space shuttle missions or at a space station. As a consequence, opportunities for materials science in space are very few and far between. Each experiment needs years of intensive preparation and can be regarded as a 'single shot' experiment with a high risk of failure. In this sense, the kind of ongoing experimental programme, familiar in materials science on earth, does not exist for materials science in space.

Nevertheless, previous microgravity experiments have shown a series of important scientific results. In the following some relevant examples are mentioned:

- In relation to microstructure formation during *columnar alloy growth* no comprehensive and systematic study exists and the data available is only limited. Using a binary transparent alloy acting as a model substance for non-faceting solidification, earth experiments show deformed interfaces and do not allow quantitative pattern evaluation. In contrast, the space growth sample shows an undisturbed and rather regular hexagonal pattern with fewer defects (Fig. 2.26). Directional dendritic solidification under conditions of purely diffusive heat and mass transport conditions in space show significantly regular patterns consisting of larger dendrites in the space experiments (Fig. 2.27).

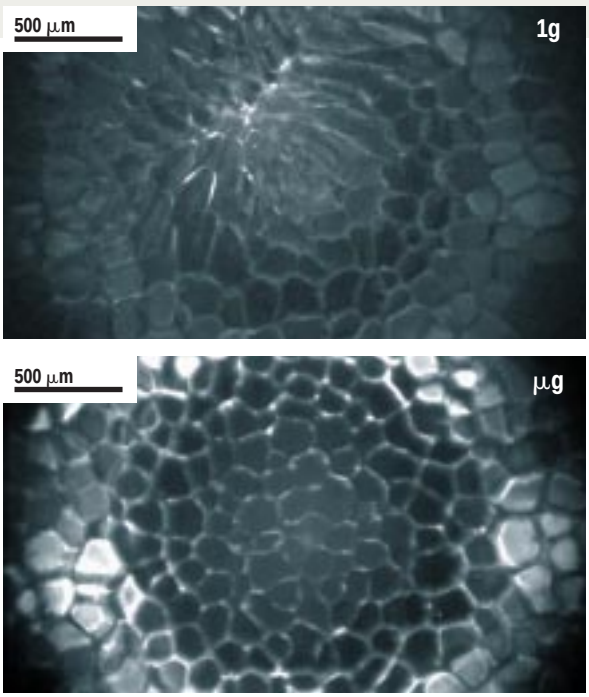

Fig. 2.26. Top view of a cellular solid-liquid interface in a transparent succinonitrile-0.075wt%acetone alloy, directionally solidified at a temperature gradient of 2.2 K/mm and solidification velocity of 2.5 µm/s. The interface structure of the earth-grown sample (upper picture) is greatly interfered with by convective buoyancy flow in the melt. The cellular morphology in the space-grown sample (lower picture) is much more regular and allows fundamental investigation into morphology evolution (ACCESS).

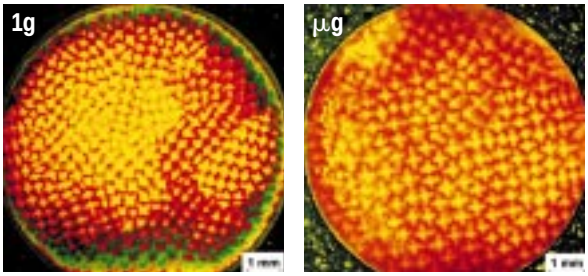

Fig. 2.27. Cross-sections of directionally solidified Cu-29.5wt%Mn samples at a temperature gradient of 2.75 K/mm and solidification velocity of 5.8µm/s. The dendritic morphology of the space-grown sample (pictured right) is more regular and shows dendrites approx. 30% larger in size. These findings are attributed to the conditions of purely diffusive mass and heat transfer in the melt in the microgravity environment (ACCESS).

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- First experiments in space in the field of *equiaxed growth* confirm an environment free of sedimentation. The resulting grain structure is much more regular than on earth (Fig. 2.28) and will provide a starting point for a better understanding of grain growth mechanisms. Sedimentation-free solidification is also important in the case of peritectic systems which exist for many multicomponent alloys. Solid peritectic phases grow in the melt and behave like *in situ* particles. The diffusive growth conditions obtaining in space allow undisturbed observation of such technically important phenomena (Fig. 2.29).

- The principal objective in relation to *crystal growth* of semiconductor materials is to study the origin of chemical heterogeneities, both on the macroscopic and microscopic level. Space experiments using InSb and doped Ge in Bridgman-type facilities show almost striation-free crystals and therefore much better homogeneity. For crystal growth without contact to the wall the floating-zone technique is used. Space experiments using Si show that surface tension-driven Marangoni convection also impacts in a microgravitational environment and restricts achievable homogeneity. On the other hand, using compound semiconductors, such as GaAs or GaSb, crystals in sizes not attainable on earth have been processed.

- Containerless processing in space allows determination of the thermophysical properties of the melt, e.g. viscosity, thermal conductivity, diffusivity, surface tension or enthalpy. In particular for glass-forming or highly reactive alloys, these space experiments provide unique data for thermodynamic modelling.

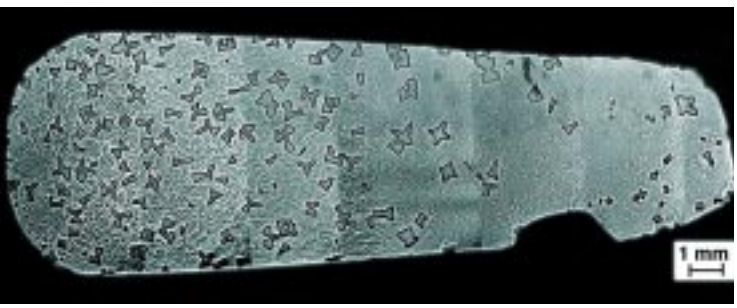

Fig. 2.29. The picture shows a cross-section of an Sn-13at%Sb sample directionally solidified in microgravity during the TEXUS-34 mission. The peritectic phase becomes directionally solidified from the left up to the marker (white lines outside), after which the sample is quenched. The pro-peritectic phase is dispersed over the whole sample because there are no sedimentation effects (ACCESS).

Fig. 2.28. Equiaxed solidification of refined Al-4wt%Cu alloys under almost isothermal conditions. The space sample (pictured right) shows a homogeneous microstructure of dendritic crystals of nicely uniform grain size. By contrast, ground samples show a much larger dispersion of grain size in the central part and an accumulation of very globular crystals at the bottom as a result of sedimentation (courtesy D. Camel, M.D. Dupouy, CEA Grenoble).

2.11.3. Expected Breakthroughs and Future Visions

Materials science in space is expected to make a crucial contribution both to the fundamental understanding of materials processes and in enhancing materials properties. Sophisticated experiments in a microgravity environment allow crystal growth or alloy solidification under purely diffusive heat and mass transport conditions. In addition, containerless sample processing available in space allows the measurement of properties of the melt such as viscosity, thermal conductivity, diffusivity or surface tension. This is why convection-free or containerless processing of this

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kind provides a unique database for enhancing the accuracy of numerical models of microstructure formation.

Fundamental investigations of this kind may result in the enhancement of industrial products. At present, there is a rather large gap between simplified scientific experiments and complex technical processes. To improve the transfer of knowledge, closer interaction between science and industry is absolutely necessary. This means greater transparency in scientific results for industry, as well as specification of specific problems as an input for scientific research using microgravity.

Two essential boundary conditions make the achievement of such a breakthrough within the next decade a realistic possibility. Firstly, within the next few years the International Space Station ISS will be providing a platform for carry out ongoing experiments in microgravity. Secondly, future activities in space will be joint experiments by groups of scientists from different countries defining a common scientific programme. Within the scope of this Microgravity Applications Promotion (MAP) programme of ESA, industrial partners are directly involved in order to define materials science research in space. In this sense, the concept of "learning for earth in space" can be realized.

2.11.4. Research Potential and Priorities

Research potential for materials science in space can be identified in areas in which buoyancy effects in the melt and sedimentation effects on earth play an important role. Space experiments allow a diffusive growth condition. Three main topics can be defined as follows:

(a) Solidification of metallic alloys

During directional solidification processes on earth, convection in the melt significantly impacts the growth structure of the solid-liquid interface. In the case of metallic alloys, the main future goal is reliable determination of fundamental relationships at microscopic scales. The strategy is based on a joint approach using well-defined space experiments and theoretical and numerical modelling. Progress is mainly required in two topics:

- In columnar growth, our understanding of the formation of non-planar solid-liquid interface patterns is nowhere near complete. In particular, understanding the stability and dynamics of dendritic or mushy interface structures, impacted by melt flow and freckle formations, is essentially important to most industrial casting processes. Benchmark experiments in microgravity allow much more ordered cellular or dendritic morphologies as a basis for a better fundamental understanding.
- Equiaxed growth often occurs in casting processes. The development of equiaxed grains in the undercooled melt can be studied extremely well through space experiments without superposed settlement of nuclei.

In particular, lightweight metallic alloys, as applied in the automotive industry, should be used for future well-defined benchmark experiments. The results obtained in such experiments will provide a database for numerical modelling and will be an aid in improving technical processes.

(b) Solidification of semiconductor materials

In the case of semiconductor crystal growth in space the main objective is to understand the role of the basic transport mechanisms in the melt, i.e. buoyancy and Marangoni convection. This is the prerequisite to producing larger-sized crystals with a greater degree of homogeneity and fewer defects than on earth. Key topics in the field of crystal growth may be wall-free growth from the melt (CdTe and compounds of Si and Ge), growth from the vapour phase (HgI_2), and research into chemical segregation in highly concentrated alloys.

(c) Determination of thermophysical properties

Most technically relevant materials consist of more than two components. During solidification, a very broad range of different phases may occur, either enhancing or drastically deteriorating the properties of the materials. Understanding and predicting the structure of multi-component alloys demands determination of thermophysical properties and knowledge as to how stable or metastable phases are formed. Space experiments using a containerless processing technique may be able to measure relevant thermophysical data such as viscosity, thermal conductivity, diffusivity or surface tension in a highly accurate way. This data is necessary input to enhancing numerical modelling of industrially relevant solidification processes.

To sum up, in the above-mentioned topics, materials science in space is expected to be of great benefit in the future, both by achieving better fundamental understanding of solidification processes and by enhancing casting technologies.

2.11.5. International Situation

Materials science in space in non-European countries is mainly concentrated in the U.S. and Russia, the two countries maintaining their own space facilities for research. At the same time, financial restrictions and the limited number

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of flight opportunities, comparable to the situation in Europe, allow only a restricted number of space experiments.

Russian scientists have been able to benefit from experiments on the space station MIR carried out over the last 15 years. Facilities for crystal growth and solidification furnaces were available. Unfortunately, published scientific results are very scarce and evaluation therefore very difficult.

In the U.S., several groups of researchers are using a microgravity environment for materials science. An important example is the equiaxed growth of a thermal dendrite into an undercooled melt. This sophisticated experiment has allowed fundamental studies of diffusive crystal growth and provides excellent data for theoretical models. A second example deals with the interaction of particles at a moving solid-liquid interface. Mechanisms of particle pushing or engulfment are studied without the effect of sedimentation of particles in the melt due to different specific densities.

To sum up, the boundary conditions for materials science in space throughout the world are comparable and there is no intensive and ongoing research. More so than in the past, in the near future international scientific cooperation must be established to work out a common definition of the most relevant topics of research, and also to carry out series of experiments on the ISS, sharing the results between the various players. The Announcements of Opportunity for Space Experiments on an international level can be cited as an example.

This will make materials science in space a concrete example of international scientific cooperation. The most relevant topic for fundamental and application-oriented research will be defined by international groups of scientists. The experiments will be carried out, evaluated and published by international teams. Thus considered, the project is part of the vision of a global world.

Conclusions

In this chapter a number of areas of materials application were described in terms of specific examples. These applications help our modern society function and will play an increasingly important role in the 21st century. Several scientists have declared this century to be the century of biology and biomaterials. Great advances have already been made in the field of biomaterials and biomimetics. However, this research has usually been carried out by engineers rather than by scientists. Consequently the materials in use today have some desirable properties but they were not developed specifically for biological applications. It was and still is difficult to understand the interaction between biomaterials and natural tissue. The solution so far has been to cover conventional materials with hydroxyapatite, which has excellent mechanical properties and reduces the problems of toxicity. However, the lifetime of these biological materials is limited, ranging from 5 to 10 years. Second generation materials have to be developed via close collaboration between mechanical engineers, theoreticians (esp. computer modellers), materials scientists, biologists, chemists, physicians, and surgeons. A strong link to the appropriate industry is, of course, also required. However, there is the usual problem of commercial competition and barriers to the free flow of information. It is important that fundamental research into biomaterials receives a strong push similar to the way solid state science did some 40 years ago.

An interdisciplinary approach to fundamental research should result in major breakthroughs in the generation of new biomaterial components. These components should be able to replace human organs and body parts and have low rejection rates and high durability. A similar challenge is to understand biology via a biomimetic approach. The results of these studies will be used to generate artificial materials that can be applied in different areas. It is well established that biological cells are built from macromolecules and supramolecular assemblies. Both the intracellular architecture and the interaction between cells are based on soft and flexible nanostructures that are multifunctional and highly intelligent materials. In addition, cells are able to build up hard materials such as shell and teeth and to control their morphology on the nanometre scale. Several challenges await research into biomimetic materials research, including understanding of the material and transport properties of biological cells and tissues.

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Furthermore, it should be possible to construct a model system to which one can apply the experimental and theoretical methods of physics and chemistry. The results of experiments should be used to confirm or build on this model so that it can be used to develop better materials. If detailed knowledge is obtained from the biomimetic approach, it can be used to develop new types of designed materials that are biocompatible and have well defined physical, chemical and biological characteristics. These materials could be used in bioengineering as well as in pharmacology and medicine. This objective again requires a highly interdisciplinary approach.

Materials are also critical to catalysis. To date, both homogeneous and heterogeneous catalysis have been based primarily on empirical knowledge, which is now reaching its limitations. Considerable effort is needed to replace these empirical-based systems with a more theoretically grounded approach and start a *de novo* design of catalysis. This again requires strong links to be formed between physical chemistry, inorganic chemistry and chemical engineering.

Other materials with specific properties have to be developed by fundamental research (e.g., optical, magnetic, and superconducting materials). Impressive progress has been made over the last decade, also within the 5th Framework Programme, and quite frequently on a phenomenological level. More fundamental research has to be done to overcome specific barriers. One example may be the optical properties of fibres. There are enormous challenges facing the development of new optical fibres with the required complex array of properties. An optics equivalent of Moore's law also exists which says that the capacity of one fibre increases by 33% every year. This law can only continue to be obeyed if new materials and new processing routes are developed.

Similarly, magnetic and superconducting materials research can only be furthered if metallurgists, physicists, chemists and engineers collaborate to understand the fundamental factors determining these materials' properties. A comprehensive theory of superconductivity is still needed to understand why high T_C superconductivity occurs in cuprate ceramics. Nevertheless, it is well established that for real materials the critical parameters of superconductivity are controlled by the microstructure of the material. A deeper understanding of the processes, however, would also be of great utility. Controlling the microstructure during processing is essential.

This is also true for materials used in nuclear fusion and transportation. A diverse range of materials is used in both these areas for a host of different functions, so that interdisciplinary research is indispensable. For transportation it is also important that the economic and ecological aspects are taken into consideration.

Materials science in Space leads to an understanding of the influence of gravity on different aspects of materials, particularly their processing. This research is of both fundamental and practical interest, especially if specific materials with well-defined microstructures have to be synthesized. This type of research should lead to a better understanding of specific processing conditions and phenomena.

A major challenge will be the development of materials that fulfill not only one function (application) but also different functions; so called multifunctional materials. The combination of different structural and functional properties in the one material will play an important role in the future, especially in the form of nanomaterials.

An often overlooked aspect of choosing materials for applications, especially new materials, is the need for wider dissemination of research results and properties to engineers and others in industry. Creation of databases, use of the Internet, and distribution of materials journals to a wide audience all play a role in shortening the time between the discovery and application of a material.

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3. Innovation in Materials Science by New Interdisciplinary Approaches

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Introduction

Materials science emerged as a independent interdisciplinary science in the 1950s. It encompasses traditional fields such as metallurgy, ceramics, polymer science, physics, solid state physics, and solid state chemistry. At first, materials science was conceived of as an intradisciplinary approach, where the different disciplines collaborated for just a specific time on a specific problem. However, the interaction between the traditional disciplines proved to be very fruitful and continued to increase. Scientists from the different disciplines soon learned that the concept of materials science as a whole required interaction with all the different fields. In this way, materials science quickly turned into a very successful field in and of itself generating new materials essential for advancing energy, transportation, and information technology.

Materials science departments usually include different groups representing the base disciplines in science such as chemistry, physics, physical chemistry, and engineering. The synergistic effects of the close interaction have become quite apparent. For example, many of the advances in technology such as rapid information exchange, rapid transportation, and fuel-efficient aircraft are a result of strong interdisciplinary interaction.

In addition, huge progress in materials research has been made as listed in Table 3.1.

Successful Research in Materials Science
• Metallurgical research
• Microstructure and mechanical properties of metals
• condensed matter physics and materials research
• Quasiperiodic crystals – a revolution in crystallography
• New and artificially structured electronic and magnetic materials
• Materials research in catalysis
• The role of chemistry in materials science
• Advanced ceramics
• Organic polymers
• Surface science
• Materials synthesis and processing
• Nanotechnology

Table 3.1.

◀ α- and β-phases in the high temperature alloy Nb-32%Al-8%Ti viewed in polarized light (U. Täffner, MPI für Metallforschung Stuttgart).

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Each of these areas represents a part of materials science. For this reason, the major part of this White Book on fundamental research in materials science is devoted to the interdisciplinary relationship of the so-called traditional fields, i.e., those that cover the fundamental disciplines of physics, physical chemistry, and engineering.

However, it has become quite obvious that we need to broaden our understanding of the field of materials sciences to also include other disciplines, such biology, medicine, information technology, and nanotechnology.

Thus, the following sections provide a few examples where the field of materials sciences has successfully incorporated aspects of biology, medicine, and quantum computing. In addition, several studies are available that consider the expansion of the interdisciplinary field by adding more disciplines (i.e., introducing intradisciplinary activities in the areas of polymer science, information technology and nanoscience).

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3.1. Present State of Materials Science

In the last fifty years materials science has been characterized by a remarkable structural change. Materials science was born in the scientific community of engineers, in the middle of the last century. The success of solid state physics and chemistry opened opportunities to build various bridges between materials engineering and the natural sciences. The penetration of the new thinking occurred with different speeds in the various fields, for instance very rapidly solid state physics and materials science were interconnected in the semiconductor research. A similar successful interlinking was developed between materials science and polymer chemistry. In other fields such as the development of structural materials, the higher complexity of the dominating processes required the coverage of all length scales from the microscopic via the mesoscopic to the macroscopic properties. It took much longer to implement basic models discovered in physics or chemistry. For some applications new mathematical concepts had to be worked out first, like the renormalization theory for the description of phase transitions, the J-integral concept in fracture mechanics, the concept of fractal geometry for the understanding of cluster growth and colloidal systems, or the solution of the non-linear moving boundary problem for Laplacian growth processes to explain morphological phase transitions. Now at the end of the 20th century this development is mainly successfully completed. The advanced materials science has been established as discipline at the crossing point between engineering, physics, chemistry, and mathematics (Fig. 3.1). In this process specific theoretical and experimental approaches have been created which depend on concepts of both, engineering and natural sciences.

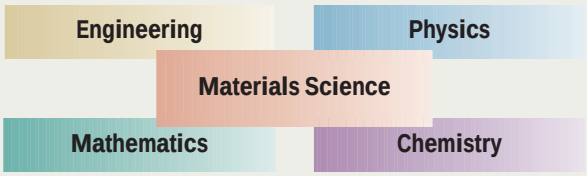

Fig. 3.1. Materials science has been formed at the crossing point of engineering sciences, physics, chemistry, and modern mathematics.

3.2. Multidisciplinarity in Materials Science

Materials science is a crossover between various fundamental disciplines such as solid state physics, chemistry, mechanics, and process engineering. Recent developments in materials science and other related disciplines have made multidisciplinarity a key issue.

The need for a new approach will be obvious when we consider the reduction of the scattering of properties – a challenge for the next decade, as far as structural materials are concerned. Rather than improving the average property, which sometimes has reached its physical upper limit, it is essential to reduce the dispersion. Controlling the dispersion means understanding (i) the effect of process parameters on the variability of the microstructure, and (ii) the quantitative relation between these microstructures and the resulting properties. Classical materials science aims at answering to these two questions. In contrast, process engineering will proceed by statistical analysis, and will improve through the use of Artificial Intelligence (AI) techniques such as fuzzy control, or neural networks. Understanding and controlling the dispersions in properties of materials will certainly imply a close collaboration between these two approaches, requiring a neural network partially trained on fundamental scaling laws of physical metallurgy. The development of such tools requires a close collaboration between materials scientists, process engineers, and applied mathematicians.

Over the past few years, a clear trend in structural materials is the use of materials processing to evaluate and predict a component's lifetime. Problems such as joining materials, casting defects and their influence on the lifetime of the materials are key issues from an application-oriented point of view. Those problems also require further scientific investigation from many specific angles: for instance, it is only possible to study hot tearing in cast components or in welds through a close collaboration between specialists in thermodynamics, solidification and micromechanics.

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For new emerging fields it is crucial that the required research is approached in a multidisciplinary way. This chapter briefly discusses the following three fields: (i) design of materials components, (ii) recycling of materials and (iii) biomaterials science.

The field of *design*, which means a selection of optimal materials and processing for industrial applications, has seen a complete revolution in the last ten years with the occurrence of new systematic methods to compare materials and processes in an objective manner [1]. These methods have proven their efficiency because it was possible – with the availability of high-performance computers – to implement them in *software programmes* and to handle huge amounts of data, structured in databases, for multicriteria selection. The evaluation of the costs of the different processes was based on comparing them on the basis of a microeconomics model. This booming field of «selection guides for design» is an impressive example of multidisciplinarity in materials science. The most recent developments in this field cover the systematic investigation of all possible applications, and in the near future these developments might direct the development strategies for new materials. Such an approach is simply impossible within a narrow separation of different scientific domains.

Recycling is becoming a crucial issue. The current overwhelming importance of *ecological* aspects in industrial and political decisions has important consequences on the development and selection criteria of materials. Solving this problem requires skills used in various fields, including (i) physical techniques to separate different qualities of wastes, (ii) investigations of the biological or chemical mechanisms for their remediation, (iii) problems induced by the recycling (Fe impurities in Al alloys, Cu embrittlement of steels etc.). Recycling is a source of interesting problems for materials scientists, but the science of recycling has still to be created. This field would integrate the technical, economical and sociological needs in a systematic approach.

The educational system in Europe still relies on two paradigms: the classification of sciences by Auguste Comte, and the hierarchy course/tutorials/practicals in our pedagogical practices. The need for multidisciplinarity will force an evolution of the educational system in these two areas.

Rather than trying to remove existing barriers between disciplines, we should consider an alternative approach: just not building them. Project work should reacquaint students with the fact that scientific methods are universal, and the various sciences are not subordinate to each other, but all of them rely just on specific scientific methods. If we want the next generation of scientists to be able to generate new fields in materials science and work on these new scientific challenges with innovative minds, we have to train them in two ways: a technical approach to science which is the current methods, but also a cultural approach to science, which will develop their inquisitiveness.

3.3. Obvious Needs for New Ideas

One of the most important contributions of physics and chemistry to materials science has been the microscopic understanding and design of new materials. Together with appropriate new analytical tools, such as high-resolution electron microscopy, synchrotron radiation, high-resolution mass spectroscopy etc., and by new processing methods on the atomic scale (e.g. by scanning probe methods, lithographic methods, or the synthesis of supramolecular structures etc.) this microscopic approach created a completely new world of artificial materials with properties controlled on the nanoscale [2-4].

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3.4. Important Topics in Scaling of Materials

3.4.1. Design of Small-Scale Structures

The unparalleled performance of today's computer technology was enabled by revolutionary changes in microfabrication technology. In particular, the down scaling of characteristic feature dimensions of electronic components from a few microns to a few tenth of a micron allowed the realization of processors with ever increasing operating frequencies. During the last decade design ideas and fabrication methods from the world of microelectronics have started to inspire other disciplines. As an example consider the popular field of MEMS (Micro Electro Mechanical Systems). MEMS take advantage of existing microelectronic fabrication techniques for creating miniature sensors (e.g. accelerometers), and microactuators (e.g. valves, mirrors). Such devices may ultimately lead to improved performance such as increased power density, improved system reliability through component redundancy and *in situ* monitoring of critical components. Novel processing methods such as MEMS and Solid Free Form Fabrication will have to be significantly improved to allow the construction of objects with unprecedented shape resolution, dimensional tolerance and complexity.

Materials research will be a key element in the realization of new miniaturized devices. The variety of materials, that can be processed with microfabrication techniques, ranges from plastics to metals to ceramics and is expanding rapidly. New high-performance materials will urgently be required for small engines, microfuel cells, embedded microsensors and actuators. These may be developed following entirely new engineering design principles, including the use of materials in applications where they could not be used previously. System redundancy may for example allow the use of brittle materials in mechanically loaded systems. Furthermore, such new fabrication methods may also lead to the manufacture of novel materials, e.g. with negative coefficient of thermal expansion or negative Poisson's ratio. It is immediately clear that materials and design issues are intimately connected to the development of micro-components and need to be addressed together. This will require the cooperation of materials and mechanical engineers, to an even greater degree than in today's development of large-scale components.

3.4.2. Interfaces and Surfaces

As structures become smaller, surfaces and interfaces gain in importance with an increasing surface-to-volume ratio. We need to develop, therefore, greater understanding of the relation between structure, thermodynamics and properties (diffusivity, reactivity, segregation behaviour, equilibration conditions) of surfaces and interfaces. Surfaces and interfaces obviously dominate adhesive and frictional properties of small-scale materials. In particular, they also affect the number and configuration of dislocations and therefore the plastic response of a material. For example, dislocation cells, the formation of which is still not completely understood even in the bulk, will also be affected by the presence of surfaces through image stresses. This can make the creep behaviour of thin films substantially different from that of the bulk material. With decreasing grain size the Hall-Petch relation of the yield increases. This leads to a qualitative change as the number of dislocations in pile-ups becomes small. Multilayered films and consolidated nanocrystals give contradictory results here.

A common weakness of small structures is their limited thermal stability. The reason lies in the fact that kinetic materials processes are size-dependent on a variety of scales. Examples are the equilibration of surface and interface shapes, the interfacial reactions (including the formation of non-equilibrium phases), and the formation of mesoscopic interface structures such as ledges. Assessing thermal stability of metastable structures requires detailed understanding of the interfaces involved in nucleation processes. The main unknown is the energy of the interface between a second phase nucleus and the matrix. The determination of this energy is particularly challenging for the case of nucleation from a liquid, since the interface is difficult to access experimentally, and modelling of its structure and thermodynamic properties is complex.

Organic thin films are in many ways different from metallic or ceramic ones. By constraining a polymer to a thin film, its conformation can be quite different from that in the bulk. Organic monolayers, often self-assembled, either on a substrate or as a membrane, have unique structure, thermodynamics and mechanical and functional response. They can also be used to coat small particles and thin films to induce functionalization and self-assembly. Research along these extremely promising lines is only in its infancy.

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3.4.3. Understanding Materials Across the Length and Time Scales

An important issue in materials science is how mechanical properties such as strength, hardness and toughness scale with the characteristic size of a microstructure. This issue is especially important for materials problems in micro- and nanotechnology. Computer modelling has become an indispensable instrument for the advancement of the theoretical understanding of materials, particularly for small-scale materials and systems, where the magnetic, electronic or mechanical properties directly depend on the internal (microstructure) and external (shape) structure. Particular attention has recently been directed towards the question whether and how the properties of a functional system can be predicted on the basis of its known atomic or molecular composition (see Fig. 3.2). This depends on the understanding of how a particular crystal defect or a particular molecule contributes to the collective materials properties and the function of the system. This is a challenging question, that requires the connection of different modelling schemes on significantly different length and time scales. Many fundamental aspects of such a connection remain to be explored, particularly for the connection between discrete (atomistic) and continuous models.

For example, new concepts of strain gradient plasticity lead to a linear scaling law between the square of indentation hardness and the inverse of the indentation depth. Amazingly, further experimental data show that such linear scaling law remains valid even down to nanometre length scales. As a second example, it is known that fracture energy varies significantly with the thickness of metal layers in the layer structures of a microelectronic device. In this case, the scaling of fracture toughness with the characteristic dimension requires interface fracture modelling that is separately from plastic deformation in a confined metal layer. In both cases, combined efforts in theory and experiment lead to a good understanding of small structures' mechanical behaviours. Future studies are required to study a variety of material and geometric lengths and their effects on mechanical properties in small systems.

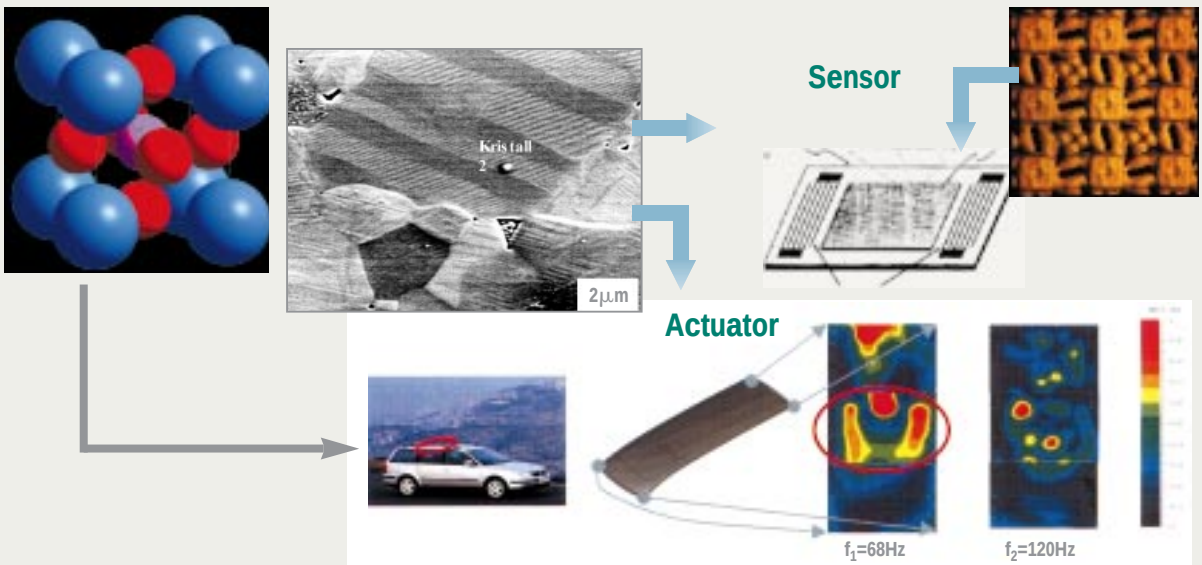

Fig. 3.2. Piezoelectric ceramics (PZT) with application as damping components in advanced cars or as substrates for new biosensors (surface acoustic wave sensor functionalized with a protein membrane) are examples for chances and challenges of materials development across the scales.

3.4.4. Simulation of the Transition to Smaller Scales

Experimentation and simulation are equally important to advance the understanding at this transition between different scales and different phenomena. In particular, *in situ* experiments geared towards testing modelling predictions will be of greatest need. This need is generated (i) by the fact that the small-scale structures are usually metastable structures, far away from equilibrium where transient behaviour is of outstanding importance, (ii) the modelling of scale transitions usually involves multiple phenomena which cannot be separated and therefore have to be compared directly to *in situ* observations.

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Examples where the combination of *in situ* experimentation and simulation may be particularly fruitful include the study of the deformation and the development of crystal defects in small volumes, their interaction with surfaces and interfaces. *In situ* deformation in the transmission electron microscope or mechanical testing inside a scanning probe microscope will give basic information on nucleation and interaction of crystal defects which are the basis for the theoretical modelling of the mechanical properties, plasticity, fracture and fatigue of small scale materials. Similarly, recent advances in micro-focus X-ray diffraction or *in situ* microscopy techniques enable materials synthesis or deposition processes to be studied; this will allow validation of computer simulations of the microstructure formation, of nucleation and growth phenomena. Considerable research effort is, however, required to reach these ambitious goals.

3.5. Learning from "Mother Nature"

At the same time we have learned from other fields that the gap is permanently growing between the materials we can artificially manufacture, and the materials we would like to produce for use in our daily life. This is evidenced in the incredible demands formulated in informatics for new materials in order to guarantee the further increase of the storage density in microelectronics. Similar challenges have been formulated for the materials science community by the life sciences. For instance, whereas in the past it was possible to satisfy the surgeons´ interest in new bone-replacement with high-performance structural materials (such as titanium alloys, cobalt chromium superalloys, or alumina ceramics), a growing number of molecular biologists, biochemists and physicians are now aware of living-tissue cellular interactions with artificial materials, a trend which clearly calls for a paradigm shift with respect to artificially manufactured tissue. Thus the question of tissue engineering arises: will it be an object of future materials science, or is it too far away from materials science approaches?

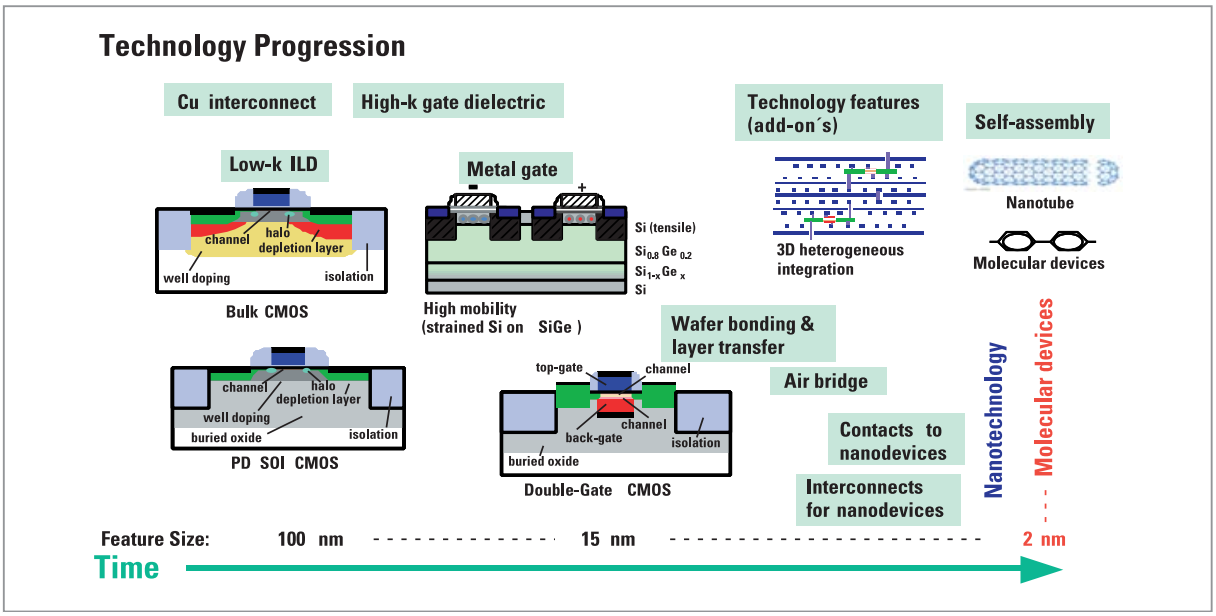

Fig. 3.3. Top-down and bottom-up approach in microelectronics to overcome the 30 nm barrier.

At this point it is necessary to ask "What could be the main difference between an artificial and a biological material?" At least one difference is immediately obvious, when we consider the building blocks of biological materials (such as proteins, carbohydrates, lipids, or DNA) and materials traditionally developed by engineers (such as metal alloys,

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ceramics, or polymers): the complexity of the living building blocks is significantly higher. The natural evolution over millions of years led to selection of very "smart" molecular structures which could be self-assembled to form the living matter. In other words "Mother Nature" uses highly smart molecules to create her objects by relatively simple and robust processing routes, whereas traditional materials science usually applies sophisticated processing routes to create artificial materials from simple elements. This situation will be transparent when we consider as an example recent developments in nanotechnology (Fig. 3.3).

There are two complementary approaches: bottom-up and top-down processing. In the first process single atoms or molecules are manipulated to create new nanoscale components. In the second, lithographic techniques are used to size down the structures to a smaller scale. The main disadvantage of the first approach is the serial processing, whereas at least today the second strategy demands enormous technical efforts to achieve sizes smaller than 30 nm. Biomolecular structures open new possibilities. Biomolecules possess dimensions typically from few to hundreds nanometres. That means, a single molecule could be used as a template, compartment etc., for the synthesis of nanomaterials. Moreover, often biomolecules can self-assemble, thus parallel processing of higher ordered structure is a characteristic feature. We see the future of materials technology as the combination of two developments:

- The convergence of top-down and bottom-up processing to overcome the 30 nm barrier.
- The connection of traditional semiconductor materials (Si, SiO_2 etc.) with organic/biological materials, possibly with 'small scale structured' interfaces.

This path would open up plenty of new technological fields.

3.6. Option for a New Interdisciplinary Approach

Molecular biology is moving into the post-genomic age. The genomes of several organisms have already been completely sequenced. Thus molecular approaches can be developed for the study of functions of cells, tissue, and organs. Growing understanding of the biological causality chains on a molecular level will open the door to revolutionary developments in tissue and organ replacement (Fig. 3.4).

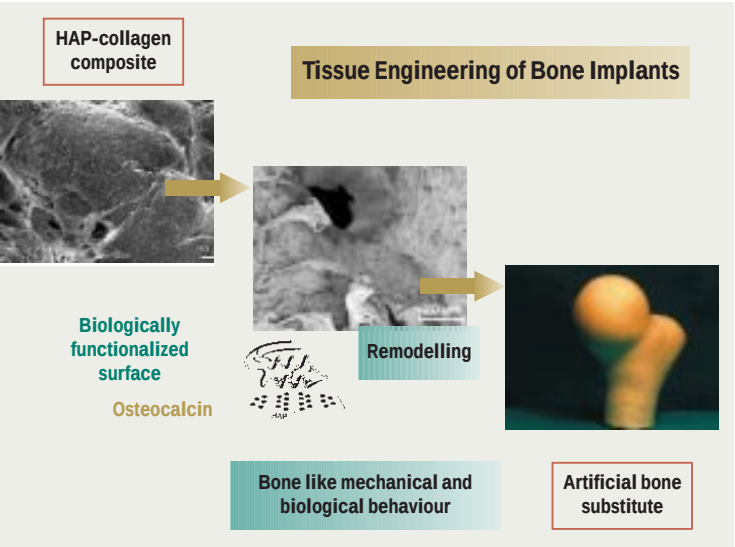

Fig. 3.4. Future processing route of materials for bone replacement – *in vitro* remodelling of a scaffold of hydroxyapatite and collagen by bone cells.

This also applies to the use of biological processes for technical applications, particularly to the development of bionanotechnology (see Fig. 3.5), and the future manufacturing of nanomachines modelled on cellular machines.

In the last 20 years it has been demonstrated that materials formed in nature have peculiar features [5]. The detailed study of biomineralization in different living organisms has shown that the smartness of the biomolecular structures and the complexity of cellular processes create processing routes to make metastable crystalline phases, nanocrystalline inorganic- and organic composites, single crystals of highly complex shape etc.. The processes are occurring in aqueous solution near room temperature, which means that they are sustainable *per se*. Increasing understanding of the mechanisms that control these processes has been obtained. Although there are still many open questions, biomimetics is already an important focus of activity in the materials science community [6].

Nature can also inspire materials research in the creation of optimized interfaces and surfaces. In a rather counter-intuitive way, finely structured sharkskin was found to

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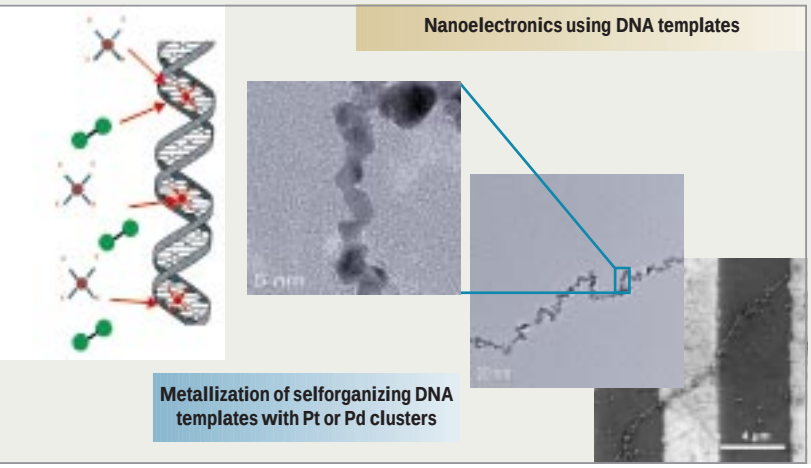

exhibit better hydrodynamic behaviour than perfectly polished surfaces. Similar surprises occurred in the search for non-wetting surfaces ("Lotus effect"). In the field of microtribology, optimally structured surfaces were found in insects that could guide the development of microstructured reversible adhesive contacts. Overall, it is obvious that the interaction between biological and materials research will very likely produce exciting materials innovations in the future.

Fig. 3.5. DNA can be used as a template with unique self-assembling behaviour to grow nanoscale metallic wires by metalization from aqueous metal complex solution.

3.7. Molecular Bioengineering – a New Challenge for Materials Scientists

Initially developed with the goal of mimicking biological processes in a completely artificial way, biological elements are now included as biomolecular templates and compartments, as well as living cells in biomimetic processing (Fig. 3.6). A promising sign is that European research groups (UK, Italy, Austria, and Germany) play an active role in developing this field together with U.S., Japanese, and Israeli groups.

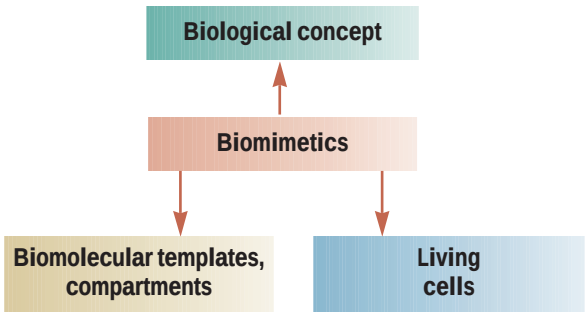

Fig. 3.6. The main elements of biomimetics. It is a hopeful sign that European research groups (UK, Italy, Austria, and Germany) play an active role in developing this field together with groups in the U.S., Japan, and Israel.

More generally, biomimetic materials processing is leading to a new interdisciplinary forum which could be called molecular bioengineering. We see three major roots for this new discipline: (i) molecular cell biology with contributions from genomics and proteomics, (ii) materials science, and (iii) bioinformatics/biomodelling (Fig. 3.7).

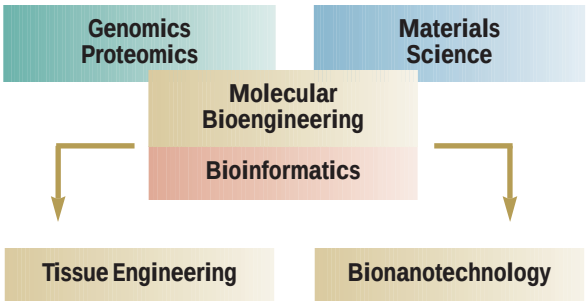

Fig. 3.7. The major roots and implications of molecular bioengineering.

The fast developments of the genomic and proteome analyses open completely new possibilities for a directed intervention in cellular structures and processes. In the creation of the new discipline "molecular bioengineering", biophysical and biochemical methods have to be incorporated into the tool kit of materials science as shown in Fig. 3.7. This development must be based on a significant broadening of academic and educational programmes. Interdisciplinary teaching programmes were recently developed at leading U.S. universities. Such programmes should be created at European universities too, with a strong background in materials science and biology. To foster this, particularly in the bioinformatics/biomodelling area, the mathematical tools have to be created to deal with the enormous data sets and to predict possible experimental strategies.

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3.8. Expectations for the Near Future

The interaction of molecular biologists, materials scientists, and bioinformatics will create absolutely new ways for materials processing. For instance already today molecular biologists can "genetically" design new protein templates or microorganisms that show highly specific binding behaviour to a given inorganic compound. "New organisms" can be created via a directed expression of genes, which code proteins that bind a specific inorganic compound. In this way the horizon for future application of biomineralization and bionanotechnology will be expanded considerably.

3.9. Actions that have to be Undertaken

- The field of small-scale materials and structures is particularly promising for creating scientific and technological breakthroughs and innovations. Studies of size-effects on the behaviour of materials and the functionality of systems are at present only in their infancy and will require substantial research efforts. Further progress in this area will critically depend on close collaborations of materials scientists with physicists and mechanical engineers, on the one hand, and bioscientists, on the other. The EC should support focused research and development programmes of cross-disciplinary teams in this field.
- The European materials science community should be allied with leading institutes in molecular cell biology and bioinformatics, to establish joint European Research Centres in Molecular Bioengineering supported by national and EC funds.
- To strengthen the research expertise, and to increase the competitiveness with the U.S. and Japan in the next ten years the EC should fund Mobility and Training Programmes in Molecular Bioengineering for PhD students and postdoctoral scientists.

Moreover research platforms in important areas of materials science should be initiated. Possible themes include:

- "Small-scale materials science and engineering"
- "Bioengineering of bone and cartilage"
- "Materials processing on biomolecular templates"
- "Cellular machines and bioengineering"

Conclusions

Materials science is by definition an interdisciplinary field. So far, the field has been an amalgamation of fundamental natural sciences disciplines such as chemistry, physics, physical chemistry, and engineering. However, recent demands from industry as well as society require that new fields be added, generating new areas of interdisciplinary research.

Research in Europe should use its chance to join highly competent research teams from materials science, mechanical engineering, physics, chemistry, biology and medicine to become a pace maker in the fast developing new multidisciplinary research fields. Cross-disciplinary interaction should be promoted by Research Networks, dedicated research platforms as well as multidisciplinary mobility and training programmes for PhD students and postdoctoral scientists. The "Research Map" for multidisciplinary activities in materials science within the EU for the next ten years is proposed, see Fig 3.8.

Chapter 3 particularly illustrates (although it is discussed throughout this White Book) that "interdisciplinarity" is the most important aspect of materials science. It is important not to just collaborate but also to develop a common "language" and common thinking. Strong interactions have to exist between the collaborations. Continuous communication between different scientist will result in fast advances. A workshop recently sponsored by the National Science Foundation and the Department of Energy on Interdisci-

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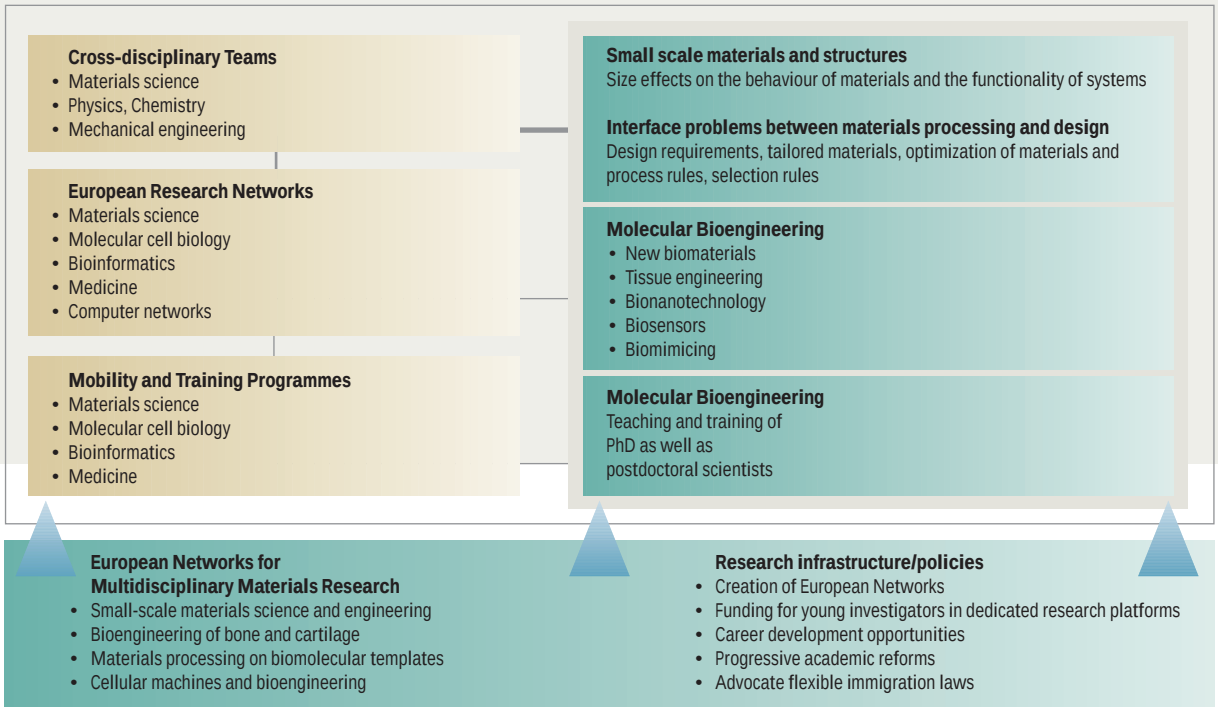
Fig. 3.8. Research map for multidisciplinary activities in Europe.



plinary Macromolecular Science and Engineering highlighted the expansion of this interdisciplinarity by the addition of the field of macromolecular science to the materials sciences arena. Large molecules can be considered the cornerstones of complex biological systems that were formed by evolutionary processes that went on for million of years. Techniques developed in physics and chemistry can now find use in the macromolecular science and engineering disciplines, particularly with regard to such biological structures as genes and proteins.

As we stand at the beginning of the new century, we can clearly see that the knowledge that is rooted in disciplines such as polymer science, chemistry, biology, and engineering is converging to initiate a new interdisciplinary field-that of macromolecular sciences and engineering. The origin of this new field is the narrow area of polymer science and engineering, which has grown over the past four decades around plastics technology. This new field could have a profound impact on society with respect to both economics and quality of life. Specifically, the field will have a strong influence on the pharmaceutical and biomedical industries, manufacturing, infrastructure, and electronic information technology. Similarly, interdisciplinary macromolecular science will play a critical role in the development of nanotechnologies since the macromolecule is the main object of structural diversity .

We can also see that specific connections between biomaterials and macromolecular biology could be very fruitful. The connection between cells and computer hardware could deliver new types of environmental sensors, medical diagnostic equipment, and probes of biological objects such as viruses and bacteria. Macromolecules hold the key to such connections because cell receptors are essentially polymers embedded in the cell membranes. Novel structures also need to be discovered to generate contacts between synthetic and biological macromolecules.

Recently, futurologists pointed out that the most important technologies of the 21st century-nanotechnology, robotics, and genetics-may generate a “machine” or an “animal” which may eventually make humans an endangered species. Although it is true that some aspects of this vision of interdisciplinary research may well be frightening it is our belief that the benefits to humankind outweigh the risks. Like the discovery of nuclear fission, which led to the atom bomb but also found numerous beneficial applications, it is hoped that mankind will be intelligent enough to use the new technologies wisely.

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4. Materials Theory and Modelling

Introduction

Theoretical modelling of materials is an important and fundamental aspect of materials science that will become even more important in the future.

Using the fundamental principles of physics and chemistry governing the states and properties of condensed matter, materials theory is devoted to modelling structural and functional properties of real materials quantitatively, and consequently to designing and predicting novel materials and devices with improved performance. The virtue and strength of this theoretical approach is its "predictive power". As one among numerous illustrative examples in the literature, the recent theoretical prediction of superhard carbon nitride (C_3N_4) has motivated experimentalists around the world to synthesize this new material [A. Y. Liu and M. L. Cohen, Phys. Rev. B 41 (1990) 10727-10734; M. L. Cohen, Mater. Sci. Eng. A209 (1996) 1-4].

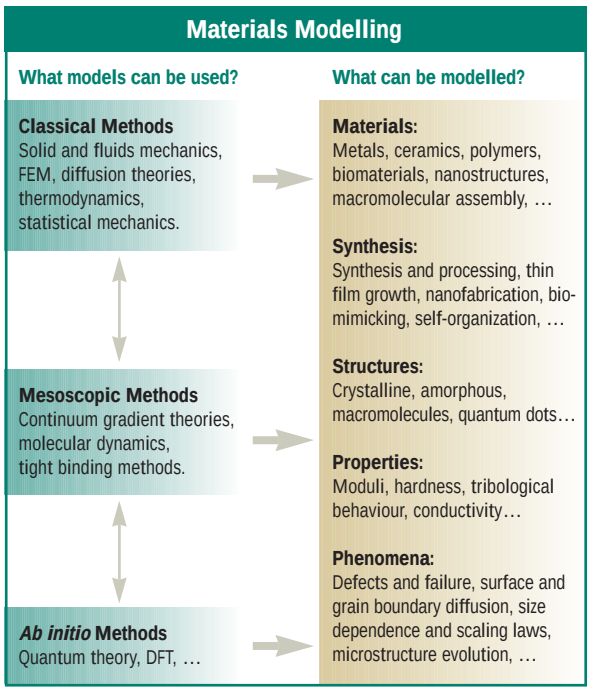

Fig. 4.1. The scope and methods of materials modelling.

Modern materials theory and modelling is characterised by the following features (see Fig. 4.1. and 4.2.):

- It is a scientific approach to technological problems:
  It aims to understand, control and design the structural and functional properties of materials for industrial products with specific purposes, lifetime and customer acceptability, distinct from theoretical studies of generic phenomena or classes of matter, as addressed traditionally in basic science of condensed-matter physics and chemistry.
- It is a quantitative approach with predictive power:
  It develops and employs mathematical and computational tools for numerical and analytical calculations. These tools are accurate, quantitative and predictive as well as robust and reliable.
- It is cross-disciplinary and synergistic:
  It uses and combines various tools ranging from practical materials engineering to fundamental condensed matter science. It intimately connects theory to experiment for the same material under investigation. It bridges length and time scales across many orders of magnitudes by judicious selection of approximations: quantum mechanics, atomistic, continuum and statistical theories.

◀ Surface of a molten Si sample (optical micrograph obtained using interference contrast, G. Kiessler, MPI für Metallforschung Stuttgart).

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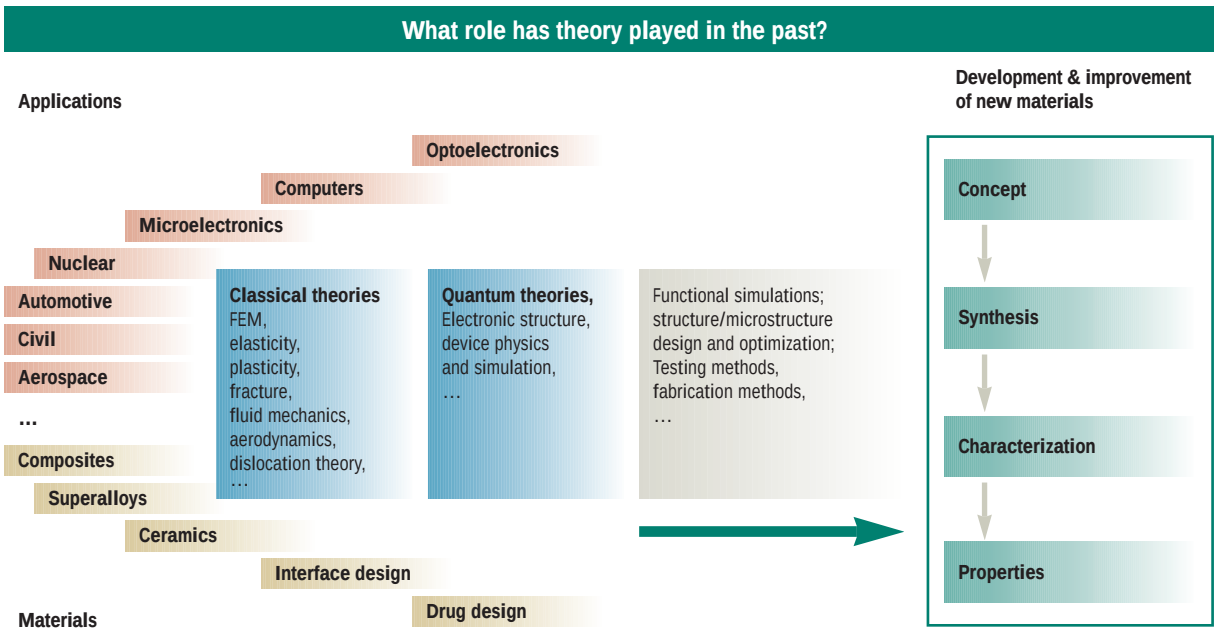

Fig. 4.2. Materials theory plays an indispensable role in the development and improvement of new materials in various industries.

Consequently, materials theory and modelling is applicable to and beneficial for essentially all established as well as newly emerging fields of interest in materials research (see Fig. 4.2.):

- molecules, crystals, intrinsic structures and properties of condensed matter, surfaces and interfaces;
- thermodynamic states and kinetic processes, chemical reactions;
- microscopic defects and nano-structured devices;
- mesoscopic structures and biomaterials.

In the following, capabilities and perspectives of this modern and active branch of materials science are illustrated with respect to three different points of view, based on the materials science of traditional solid state materials, soft matter, and nano- and biomaterials. These aspects are discussed in the sections:

4.1. Predictive Modelling of Materials
4.2. From Basic Principles to Computer Aided Design
4.3. Theory, Simulation and Design of Advanced Ceramics and Composites
4.4. Modelling Strategies for Nano- and Biomaterials

Contributors:
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4.1. Predictive Modelling of Materials

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4.1.1. What is meant by "Materials" and by "Modelling"?

Materials modelling includes familiar tools which are already part of engineering practice. These include finite element (FE) and finite difference (FD), computational fluid dynamics (CFD), and free-energy minimisation programmes. These can all be usefully extended and improved. But *Predictive Materials Modelling* goes much further. State-of-the-art electronic structure calculations can lead to cements with the right setting times, or to the best choices of piezoelectric transducers. Atomistic studies can identify the right catalyst system, or the behaviour of nuclear fuels under extreme conditions. The quantitative understanding of structure at the mesoscale and how these structures are created can improve polymers, the texture of ice cream and thermal barrier coatings. One active field, established commercially, uses quantitative thermodynamic, kinetic and statistical modelling to produce alloys with enhanced performance, e.g., improved recyclability, or materials optimised for gas turbines.

Predictive materials modelling is not new, of course. Pioneering work by Mott in the 1930s was followed by the first general-purpose codes for the semiconductor and atomic energy industries in the 1950s and 1960s. Changes in the last few years have been dramatic. This prompted the UK Foresight Programme to review the field, and especially what should be done. This present paper brings together some of what was learnt from that exercise, which was based on an e-mail questionnaire, open meetings, and extensive individual discussions.

There are very diverse views as to what "materials modelling" actually is or is not. It is not theoretical solid state physics, except as a source of methods and their validation. Apart from excluding approaches like CAD (computer-aided design), FE (finite element) methods, or CFD (computational fluid dynamics), we adopted the empirical working definition "materials modelling is that which is done by those who regard themselves materials modellers". "Modelling" includes computer-based approaches with very varied strategies, not excluding analytical methods. Its role depends greatly on the industry involved. In *drug design* the molecule (perhaps hydrated) is most of the story, and there is a large amount of "Research" relative to "Development". Modelling in a "guided choice" approach, pre-selecting favoured new molecules, leads to large economies and, to a fair degree, discoveries generate the market. Yet there is a limit: no one could licence a drug which was only computer designed. In *aerospace* there is plenty of "Development" and less "Research", since for aerospace the big issues are more about integrating many technologies, and less about exploiting some single discovery or advance. The *chemical industries* will often use CFD and other tools based on mass action and thermodynamic data. The *semiconductor industry* defines modelling challenges in the Semiconductor Roadmap (SIA1994), ranging from strain-layer phenomena, to solid state processes under electronic excitation and with high concentration gradients. This industry's band-structure codes were among the first general-purpose codes for materials modelling.

Materials science differs from condensed matter science and solid state physics because of its crucial *technological* drivers. These include (a) *Fitness for some purpose* (perhaps an intrinsic property such as a modulus, an adhesion energy for unlike solids such as metal and glass, perhaps a capability for optically-induced change, such as writing Bragg gratings in optical fibres or photographic materials); (b) *Whole life behaviour* (such as the modelling of nuclear fuel evolution in use, high temperature creep, the breakdown of silicon oxide under electrical stress, polymer degradation after disposal); (c) *Customer acceptability*, so the product can be made and sold (e.g., factors such as colour; using the phase diagram to ensure a processing route which keeps price and quality acceptable; food texture, polymer design to ensure appearance matches performance); (d) *Economic, safety and environmental aspects* (e.g., optimizing materials for radioactive waste disposal; identifying uses of new high-tech materials which, though of high cost, nevertheless lead to overall economies, like the "carbon ceramic" forms of diamond). *Materials performance* is a proper aim of materials modelling. The traditional solid state science of ground state structure and energy are only a small component.

Technological needs vary enormously and unpredictably. A number of industries (e.g., the food industry, or the defence industries) include projects over much of this wide range of modelling. The variety takes several forms: *(a) Types of material:* Metals and metal alloys; Ceramics and glasses; Semiconductors (including multilayer and nanopatterned systems); Polymers and polymer-based composites; Other soft solids (liquid crystals; colloidal matter; ice cream); *(b)*

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Which property? Magnetic (including magneto-optic, magnetoresistive); Electrical (insulator/dielectric, semiconductor, conductor, superconductor, electron emission); Optical (passive, active, like photochromics); Thermal (conduction, barrier, heat-insensitivity); Mechanical (Young's modulus, yield strength, toughness); Special (performance as a gas sensor; laser performance, catalyst); *(c) Which length scale?* From the clearly atomic, via the mesoscopic (typically, a few nanometres to microns) to the macroscopic, with these scales sometimes extensively mixed; *(d) Which timescale?* From femtoseconds to geological timescales. Many important systems are either prepared or used when neither in thermodynamic equilibrium, nor homogeneous. It is not good enough to model just an equilibrium phase for materials most readily prepared far from equilibrium, like diamond films. Modelling the means to obtain a material can be very important, especially in high value materials (diamond, photonic or microelectronic materials).

4.1.2. Types of Modelling

Materials modelling ranges from simple visualization to state-of-the-art "accurate" methods. There is no such thing as a universal "best" method: in the most effective modelling, the degree of sophistication is right for its task. So what are the aims of materials modelling? Views varied widely, and did not support some earlier views that predicting the crystal structure of the most stable form of some material was the most significant objective. Simple properties, like bulk modulus, attracted only modest interest. The ideas most favoured by industry related to the improvement of existing materials, the direction of novel materials towards a critical need in the marketplace, the close involvement with engineers and experimental scientists, and the identification of routes which one should **not** take.

(a) Modelling as a framework of understanding

Understanding of what might be important can come from an analytical idealization, possibly using a computer for specific cases or for some parameterization. The reaction/diffusion model of silicon oxidation is an example. Property maps bring together simple analytical models and experimental data to help in the pre-selection of materials according to figures of merit. Simple calculations have the major advantage of making the big ideas clear, paving the way for more sophisticated work.

One should not underestimate this level of approach. Getting the right understanding can mean better engineering solutions. For semiconductor materials, understanding of performance-limiting defects proved of far more value than subsequent detailed defect models. It enabled routes to be found to avoid critical defects (e.g., Si in the 1960s, when dislocations were the problem, or in the 1970s, when swirl defects caused difficulties, etc). One of the major contributions of modelling (at whatever level) is to help to avoid obstacles or bad routes forward.

(b) Scoping: The next stab

Scoping calculations are designed to decide which terms really matter, by making the minimal (but perhaps sophisticated) prediction of key energies and the like. Such methods are common for defect energies, for basic comparisons of different phases, or for separating out contributions of processes occurring at the same time. They can be used for looking at trends in the relationship between performance and molecular structure. They may be used to put bounds on behaviour on very long time scales. One would not wish to take a novel component into production using only materials property values from scoping calculations, yet one might well feel happy about using scoping to eliminate some potential materials, or not to follow up some idea.

There are many approaches, from simple scoping to highly sophisticated methods. Some of the best simpler methods have an excellent track record of prediction. One such class is based on interatomic potentials, especially for ionic systems (e.g., fast ion conductors, nuclear fuels like UO_2, catalysts like zeolites), where the shell model has proved a very accurate and flexible approach. Another class includes semi-empirical quantum chemical methods, like CNDO (Complete Neglect of Differential Overlap) and its successors, and also including the newer Tight-Binding approaches.

(c)"Accurate" calculations

Use the best quantum mechanics you can afford. We must define our vocabulary, since there are common, but inconsistent, uses. **Accuracy** relates to agreement with reality, and is not the same as precision, which relates mainly to the numerical precision and reproducibility of a computation. "**First principles**" and "**a priori**" are terms which are confusingly used, only appropriate for approaches at least as basic as Quantum Monte Carlo methods. We shall use the descriptor "**state-of-the-art methods**" for the widely-used Density Functional (DFT) and Hartree-Fock (HF) approaches. Sometimes, these are "**parameter-free**" when they do not involve empirical information. In practice, there are simplified versions, such as the Local Density Approximation (LDA). These may adopt hidden empirical elements, e.g., by choosing to include or omit gradient corrections. The semi-empirical quantum chemical methods are usually systematic simplifications of DFT or HF theory. Most include self-consistency (in the same sense as HF

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theory); some approaches use local charge neutrality, which is more approximate.

Implementations of these methods make significant working approximations, whether as assumptions in pseudopotentials, or in basis set. The system may not have atomic positions relaxed to equilibrium. Is a small cluster used, or is a small supercell used? If so, what is done about polarisation due to charged species: is the cluster embedded properly? Experienced workers know about these difficulties. As scientists, they usually know how to get their models right. But this is not good enough, for state-of-the-art approaches to be used seriously in an industrial setting. In an industrial setting, those involved want to be able to trust the results they generate. If different pseudopotentials give different results, or if including or not including some terms like gradient corrections makes a qualitative difference, the results may have no useful value. They may not even suffice to identify routes not to take. "Robust reliability" is an important issue.

Accuracy (how well the predictions match the real world) is another issue. A calculation is reliably accurate, if you could trust it without any experimental input (would you fly in an aircraft whose materials were designed solely using such calculated values?). Significant cases exist where the current "state of the art" is simply not accurate (e.g., O in Si). Of course, there are valuable applications of state-of-the-art methods which are less ambitious. We found that most examples using state-of-the-art methods in the materials area (as opposed to condensed matter physics) did so to interpret spectra in materials analytical methods.

Often, state-of-the art modelling implicitly assumes only ground states in equilibrium matter. However, industrial challenges are far wider. Some metastable systems have major practical value (e.g., steels). There are substantial opportunities for materials modification by exploiting excited states and, as already noted, in both these cases, kinetic issues become important.

4.1.3. Targets for State-of-the-Art Materials Modelling

Software for state-of-the-art modelling is widely available. There is a wide range of experience in its use, mostly but not entirely in the university sector. What are the targets?

(a) Target: molecules

Molecular structure codes are widely used, often in the context of drug design (which is not part of our study). Further codes are available to predict many properties of molecules, including electrical, optical, and vibrational properties. Despite many formidable successes, there are continuing reports of cases where straightforward predictions fail, e.g., giving incorrect molecular configurations. In some cases, this may be because there are different states with very close energies, or because electron correlation has to be handled at a sophisticated level. Whatever the reason, it is an obstacle to routine use of codes in an industrial environment.

(b) Target: crystal structures

As for molecules, there are some significant successes. Some of the successes are more for trends across a series of systems, rather than for absolute predictions, but that can be nearly as useful. A recent Benchmarking Exercise for organic crystal structures showed promise, but made it clear that there can often be different structures of very similar enthalpy. This raises again the point that metastable structures can be very long-lived ("A diamond is forever", it is said). Which structure a system actually adopts can be determined by kinetics, rather than energetics, for example, and modelling needs the capability to handle both classes of structure.

(c) Target: intrinsic materials properties

These might include vibrational properties, elastic constants, optical absorption spectra, and phase changes. They may include band gaps, band widths, electron affinities and carrier effective masses. Surface properties include surface reconstructions, surface energies and surface stresses. There is much activity in these areas, some very successful. Accurate prediction of bandgaps continues to be challenging; accurate predictions of energies involving changes in electron numbers (like work function) are still more difficult.

Steels are among the cases where solid state kinetics and metastable phases are of value. It is not yet possible to use state-of-the-art methods to design, say, creep-resistant steels, although simplified molecular orbital calculations have been attempted. The right problems have still to be defined, and might involve predictions for carbides and intermetallic compounds common in heat-resistant steels. Yet valuable insights and some quantitative guidance for reducing long-term embrittlement in multicomponent systems have been achieved.

(d) Target: thermodynamics and thermophysical approaches

State-of-the-art methods are targeting these topics, although it will take time for their impact to be large. No-one expressed the view that state-of-the-art calculations would replace the current, partly empirical, free energy

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approaches in the short (or perhaps even the medium) term, except perhaps for special cases.

(e) Target: local solid state properties and energies

There has been a major effort to model intrinsic defects in materials, partly driven by nuclear reactor programmes. For metals, there are successful calculations of properties of simple defects. These include models based on interatomic forces, which might be used in molecular dynamics, as well as state-of-the-art calculations which can predict thermodynamic properties. There are significant gaps in treating cascades, for which there are extreme conditions which may involve excited electrons. For semiconductors, there have been successful models at various levels. Effective mass theory continues to work with remarkable accuracy, even outside its natural range of validity. Yet there are significant gaps, especially in understanding diffusion under realistic conditions for modern processing, such as rapid thermal processing. Again, there is much to be done to understand fully the role of different charge states and of excited electronic states. For ionic solids, interatomic potential methods based on the shell model have been very successful for certain classes of problems. Some properties, like surface energies, can probably be predicted more accurately than they can be measured. Absolute diffusion rates have been calculated with accuracy. For ionic solids, the excited states have received much more attention, partly because of clear roles in photography and other special systems. However, there are difficulties with the highly non-stoichiometric systems, where there are both combinatorial and energetic problems. The electron-lattice coupling can change dramatically from one system to another, with small polaron behaviour (in which carriers hop incoherently, rather than propagate as in silicon) important in understanding materials ranging from X-ray phosphors, nuclear fuels, and colossal magnetoresistance oxides. Clearly, materials modelling has to describe an enormous variety of behaviour, significantly more varied than for, say, drug design. This is both a strength and a weakness. The strength is the aboundance of opportunities and challenges. The weakness is the range of tools and experience needed to take up that opportunity.

(f) Target: mesostructures

Approaches tend to be system-specific, albeit with a small number of recognisable categories (e.g., whether an average medium approach is acceptable, or whether many statistically-similar realisations must be treated). There is disagreement in the field as to whether all length scales need to be treated in a single code (the “spanning the length scales” issue). How different timescales can be combined is an analogous problem, especially in systems where there is history-dependence. For example, in modelling laser ablation, there is energy absorption late in a laser pulse by free carriers excited at earlier stages. The successful examples, on the whole, did not involve multiple length scales. Successful examples of mesoscopic modelling range widely. They varied from modelling plasma-sprayed thermal barrier coatings, through laser ablation, microelectronic interconnects, organic light emitting diodes, and nuclear fuel modelling, to the texture of ice cream.

4.1.4. Technology Transfer and Other Linkages

Technology transfer raises a range of issues. The links between the science base and the software industry are very good at their best, but extremely variable. On the whole, there is poor follow-up from academic code to a commercially useful code (usually meaning a well-packaged PC-based code). Unless industry's own modelling teams give a lead, there could be a temptation to concentrate on yesterday's industries, not those of tomorrow.

The links between software houses and industrial users are also very variable. This is partly, at least, because of the limitations of the small, short-lived modelling groups in industry. Small- and Medium-sized Enterprises (SMEs) in particular lack ready sources of impartial advice. Materials modelling is itself a wealth-generating industry. It is a relatively new industry, firmly based in information technology. Its customers expect from it both the right technical content and the full range of the latest IT options. For software houses, expectations of advanced graphics have been important, since the software skills and effort to produce the right graphical images are still relatively uncommon and relatively expensive. Likewise, the effort needed to maintain a code has grown to far more than a spare-time activity of the research scientist who created the first version.

Those with modelling skills are likely to be highly sought in industries both within and outside the materials area. Once trained, students with a Master's degree in materials modelling are expected to be very versatile. They will surely be in demand from the materials industry. There is some concern that they will also be in demand from other areas such as IT.

The current fashion is to suggest networking as a cure for all problems of linkage. Networks can be useful, but can be very time-demanding. The existence of a network should not hide the fact that someone, somewhere, has to actually perform useful work, and this work must itself be funded. It is difficult to establish the right degree of networking between the participants and the degree of overlap between modellers, experimentalists, and industrial-

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ists. Historically, many pioneering codes were devised in industry or national laboratories, and then developed in academia, rather than the reverse. There are very recent examples of the same routes being taken.

There is an important and growing international dimension. Governments often wish to favour their own national firms when funding research. But many of the firms that might need modelling are multinational. Others will change ownership during the life of a project. The international context cannot be avoided. Likewise, modelling and software are rapidly becoming international activities. Many of the early modelling codes, perhaps until the 1970s, were developed within a single laboratory. This led to duplication of codes with broadly similar capabilities. Code development is increasingly international, partly as a result of electronic communication. Networking with input from half a dozen countries is hardly considered worthy of comment any more. Could it be that the most efficient way to develop modelling software is through some form of open-source "e-community"? Who will take the global lead by encouraging e-communities outside the usual political boundaries, aiming to produce the best software in the shortest time?

4.1.5. Barriers to the Take-up of Predictive Materials Modelling

It is often implicitly assumed that either the computer hardware or the software will be the most serious limitation. The posing of the problem, and the interpretation of the results, were supposed straightforward. This seems wrong. Whilst major developments in hardware and software are still welcome, other factors are more limiting. Strong opinions have been voiced suggesting that the most effective modelling is tightly linked to projects, with the important calculations at the right level of sophistication. Brainware and experience, rather than software, are crucial. So what are the hardest parts? First, framing the problem in a way that could be modelled (including knowing the level of detail or precision appropriate). Secondly, understanding enough of the modelling output to give adequate answers. Thirdly, knowing the science such that the limitations of the models were understood and the value of the answer assessed. The phrases *a priori* or *first principles* do not guarantee acceptance. Fourthly, having enough confidence to use modelling to take unpopular decisions. One important use of modelling is to give early identification of what won't work. Finally, sustaining relatively long-term collaborations of sufficient numbers of people. This management factor can be addressed in several ways. One common format places very small teams of modellers (perhaps one person) in an experimental team. However, these isolated modeller(s) can be limited in range of expertise, or may find it hard to keep up to date professionally. An approach, now less common, but with a good history of effectiveness, is to keep a separate modelling group of above critical size, ensuring serious interaction with projects by proper management.

Effectiveness is a key point. Somehow, the questions asked and the knowledge gained by modelling should be linked to the activities of the organisations that create wealth or enhance the quality of life. Useful theory does not proceed in isolation. This linkage can be difficult to achieve, and usually needs receptive scientists in industry with perceptive and sympathetic managers. Various ways are being tried to achieve the link between those who model and the main project teams, but there seems to be no consensus on the best approach.

Barriers to the effective use of modelling recur. The first barrier is ignorance in industry of what is available or relevant. A related barrier is recognizing that what is available is not relevant (or not yet relevant). Software houses have a major interest in removing the barriers. Networks provide a very limited answer, limited in that they help those industries which already have quite a lot of expertise to cross the barriers. The needs are knowledge, not just information, so the World Wide Web (WWW) is far from sufficient as an answer. The third barrier is that there may be no stable industry team suitably knowledgeable to use the software, if available. Or the industry team may not have a strong enough link with academia or national laboratories to have the modelling done as a service. Why are stable teams so rare in industry? The usual assertion is "cost." But payback is rarely attributed to the modellers, especially when the contribution was to "kill" a favourite but impossible project. The fourth barrier is technical. Given a problem, often incompletely defined, can you get a useful answer in time? Do you trust your analysis of the technical problem, the working approximations, the software, and how you translated results into useful actions? Are you still sure, if you know that the solution is expensive? The fifth barrier is convincing others that your own confidence is justified. A lack of previous proven applications, and even academic disagreement over trivia, can be damaging.

4.1.6. What should be done?

Our review of the UK predictive materials modelling scene changed some of our preconceptions. When we were able to make international comparisons, similar pictures

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emerged. The problems, discussed above, suggest a number of measures to improve matters.

Expansion of appropriate courses, looking at and beyond new graduates. Mature students and those from all national backgrounds should be welcomed, without restrictive (e.g., national) grant rules. "Defining the problem" is more important than training in software use. Since trained students are valuable in many roles in industry, numbers should not be limited by perceived needs for specialists alone.

Software industries are crucial in transforming science-based codes into products for non-specialist users. Funding software development is very difficult. This must change for scientific software industries to flourish. Development should occur in whichever sector (industry, academia, national laboratory) is best equipped. International collaborations should be welcome. **Software** still needs credibility: users do not yet trust electronic structure or mesostructure calculations, and working assumptions are not intuitive. International competition drives enhancement of hardware. Publicly-funded, state-of-the-art hardware should be available to industry under reasonable conditions.

Management: Few managers in industry recognize the opportunities offered by predictive modelling. Active groups in industry are often too small and too transient to be effective. Achievements of modelling are easily underestimated, especially through filtering out flawed proposals. Longer time perspectives are needed than those readily funded.

4.2. From Basic Principles to Computer Aided Design

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Classical materials science activities in the past largely focussed on bulk properties of different materials by characterizing them experimentally and analyzing them theoretically in terms of continuum mechanics models. Condensed matter physics and chemistry, on the other hand, focussed on fundamental physical and chemical properties of systems in the condensed phase. Surface and interface science was traditionally located somewhere in between these two fields.

This "old" view has changed dramatically over the last few years. Both experimental and theoretical tools have improved considerably so that much stronger links between basic physical and chemical properties at the atomic/molecular structural level and the overall properties of the material have been established. At the same time, many different fields of modern technology, such as microelectronics, photonics and biotechnology, require controlled design and production of ever smaller structures.

In the not too distant future, we can expect that both trends, namely decreasing sizes of structures in experiment and the increasing complexity of well characterized systems, will meet! In certain areas of biophysics, supramolecular assemblies and micro-optics and electronics, this has already happened!

In this context materials theory will play an increasingly important role as it moves more and more from a description of idealized limiting cases towards an almost complete theoretical characterization of the system being investigated. To make progress in this area, coordinated efforts between researchers in many theortical subdisciplines as well as equal interplay between theoretical and experimental investigations are needed.

4.2.1. State of the Art

Materials theory typically employs a "bottom up" approach. To understand properties of complex ordered and disordered, inorganic and organic, and hybrid materials, links between the microscopic atomic structure and the macroscopic "observables" has to be established. At this point modern materials science significantly differs from the typical engineering approach, which is usually not concerned with this link but rather starts from given properties. Needless to say, both views are complementary and meet at many points. As the size of the system under consideration increases, the complexity increases significantly (the number of states typically grows exponentially with the number of molecules). However, as a consequence of the collective many body effects, certain aspects become

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even clearer or simpler. Thus a systematic investigation of generic properties beyond the chemical details of a material will eventually lead to a more fundamental understanding of its overall properties. This can be illustrated by an almost trivial example. Consider the flow viscosity of a polymeric melt, say standard polycarbonate, an important glass-forming polymer for many structural but also optical applications. The viscosity is a key material parameter for its processing. It can be written as a powerlaw $AM^{3.4}$, where A is a material and temperature dependent coefficient and M the molecular weight of the polymer molecules. This power law is generic and the same for all polymer melts. By changing the process temperature from 500K to 470K, A increases by a factor of ten, a significant technical problem. However, by also increasing M to 2M the viscosity increases by a factor of ten! Such universally generic as well as materials chemistry-specific aspects typically have a very similar influence on the overall properties. There is a complex and often rather delicate interplay between generic and specific aspects in complex materials. This is what makes modern materials modelling a great challenge, but also so exciting.

Thus Materials Theory, both analytic and numerical, is an interdisciplinary and wide field incorporating the classical disciplines of theoretical condensed matter physics, chemistry, chemical engineering, and, increasingly, biophysics. In order to understand materials beyond (re)producing numbers, it is important to combine numerical activities with analytical theoretical work over a huge variety of length and especially time scales (over more than 10 orders of magnitude!) Only this will enable us to gain a fundamental understanding of complex (disordered) materials and allow us to make the next step towards the design of new (functional) materials based on theoretical and experimental knowledge.

Since specific materials or specific systems, like supramolecular aggregates, are mostly the target of investigations, in future the vast majority of theoretical approaches will be of a numerical nature (computer simulations). An indisputable condition for success will be the supply of computer power distributed throughout the participating laboratories and sufficient CPU time at the high end (supercomputers) combined with the availability of highly qualified and motivated personnel. The latter can only be achieved with competitive working conditions and salaries.

The (mainly) numerical techniques, which are used nowadays, can be grouped along the characteristic scales of length and time they are used for. Of course the borderlines are not sharp and, with increasing computer power, are removed and shifted continuously (see Fig. 4.3).

(a) Electronic structure/quantum calculations

The general starting point is quantum many-body theory. There are a number of computational techniques which have been developed over the last several years which are now widely used tools, e.g. in catalysis research. All these methods are, however, still confined to rather small system sizes. Most accurate, but also typically only for a few tens of atoms, are the classical quantum chemical methods (CI methods, etc.). Treating the electrons quantum mechanically but the nuclei classically is done by the so-called *ab initio* molecular dynamics (MD) methods (e.g. Car-Parrinello approach), based on density functional theory (DFT). This approach, with the use of modern parallel computers, has opened a new and wider field encompassing more complicated systems such as biomolecules and catalysis

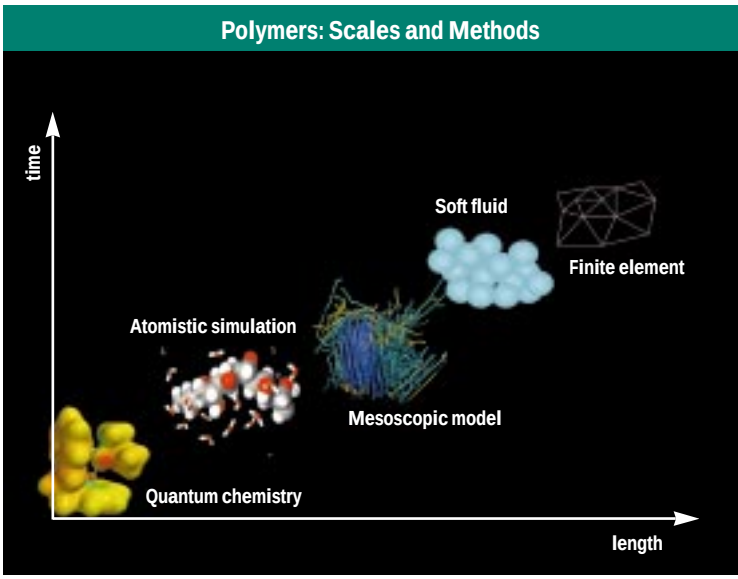

Fig. 4.3. Illustration of the characteristic scales for the simulation of polymers (Courtesy F. Müller-Plathe, MPI für Polymerforschung).

of polymers (typical system sizes are $10^2 - 10^3$ atoms, longest times about 10 ps). The next level comprises the less accurate tight binding methods. The lack of quantum mechanical treatment of the nuclei for ambient conditions is usually not so crucial. However, for many soft matter materials and for catalysis the presence of the hydrogen atoms is a severe problem. More recently new hybrid approaches which link the DFT-MD method with a full quantum chemical treatment of the hydrogen nuclei have emerged. It should be kept in mind, however, that DFT approaches generally investigate the electronic ground state of a system. For excited states, as needed for many spectroscopic studies, one has to employ a variety of quantum chemical methods. The above approaches form an indispensable basis for investigations that require specific chemical groups to be distinguished, such as in catalysis,

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catalytic pathways, specific interactions of atoms/molecules with surfaces, reactivity, crystal growth, corrosion, vibrational properties of anisotropic/disordered systems (polymer crystals, glasses...), and quantum effects in solids, to name a few.

(b) Classical calculations

To treat larger numbers of particles, an atomistic approach beyond the full quantum mechanical description of a system is needed. At this level, a classical description of the atoms is typically used. However, the interaction potentials ("**force fields**") are derived either directly from first principles quantum mechanical calculations (e.g. for surface structures) or from a combination of quantum chemical input for the (mostly) intramolecular component and experimental input as it is done for macromolecules and molecular assemblies. Current applications for these techniques range from surface physics (epitaxial growth, sandwich structures, etc.) all the way to structural and dynamic properties of liquids and amorphous solids, such as mixtures of molecular systems, synthetic and biological macromolecules, and inhomogeneous systems with complex surfaces and interfaces. Typical systems can contain up to about 10^4 atoms with typical times of up to 1 ns. For longer times and larger structural units that go beyond these limitations, **mesoscopic or generic (numerical) schemes** have been developed in recent years. The most prominent classical example is Monte Carlo simulation of the Ising model, which played and still plays a central role in our understanding of critical phenomena (phase transitions). These "coarse grained" models treat a liquid as a collection of (soft) spheres, a mesogene for a liquid crystal as a little ellipsoid or platelet and a polymer chain as a string of spheres and springs, or even as a path on an underlying lattice. The main focus here is on generic properties of rather large collections of model molecules (polymers, colloids, membranes, supramolecular assemblies, layered or nanostructural systems, alloys, etc.). Highly optimized numerical methods are available for workstation/PC-based systems as well as supercomputers. Especially for macromolecules and (supra-)molecular assemblies, this adds qualitatively new features to materials theory. The intramolecular entropy is often of the same order of magnitude as the intermolecular energies. This interplay can only be detected when both micro- and mesoscopic information is available.

To tackle even larger systems, as needed for morphology formation or many flow problems, **(semi-)macroscopic** methods have been developed. Besides the almost classical Finite Element Methods (FEM), which are widely used in engineering, new approaches have emerged. This includes a closer link of FEM to molecular properties of the underlying compound and the connection to Monte Carlo sampling for composite materials. Other methods are lattice Boltzmann hydrodynamic simulations, dissipative particle dynamics (DPD) for slow/large scale hydro-dynamics such as flow of structural liquids, nano-rheology (electrophoresis, nano-electrorheology, transport in molecular assemblies). While the latter two examples are particle-based numerical techniques, the first is a continuum approach. In between are many others, such as the various self-consistent field methods (SCF) for molecular systems.

Traditionally, these different research areas, essentially separated by length scales or time scales, have been investigated by different research communities. Massive computer power is needed to tackle these problems, but even more important is the continued coordinated effort of **chemists, physicists, mathematicians, engineers** and **biologists**. A number of national and EU-wide activities have commenced in this direction over the last few years. Such collaboration is absolutely essential to make necessary progress but also to stay competitive. This also means that sustained long term funding of the individual groups and (smaller) collaborative teams is needed.

4.2.2. Future Research and Breakthroughs

Breakthroughs depend to some degree on serendipity and cannot be predicted. However, systematic linking of the above approaches is a precondition for generating a theoretical materials science which advances from a retroactive description of systems to a discipline which provides tools with quantitative and qualitative predictive power. In the long run we should be able to make the step from molecule to nanostructure to, in a general sense, function. This will of course need not only the coordinated effort of theoreticians, but also a very close interaction with experimentalists from many different disciplines.

The most important developments can be expected in the following areas:

- Scale-bridging investigations of complex disordered materials (new basic understanding, improvement of currently used materials).
- Correlated quantum systems (quantum computing, etc.), which require new developments in nanocomposites in order to become technically feasible.
- Coatings, surface modification of inorganic materials, and use of structured organic and inorganic coatings for functional materials.
- Structure-function linking: Molecular assemblies,

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nanostructured composites for specific functions in biology, chemistry, medicine, etc.

Experiment and technology are continuously enhancing the precision of measurement and characterization methods so that structural and functional units of materials and devices can be made smaller and smaller until their physical limits are reached. At the other end of the scale, development of hardware and software together is allowing the treatment of more complex and larger units. Thus one dream of materials scientists is to eventually run experimental and theoretical (i.e. simulation) investigations in parallel in order to provide direct theoretical interpretation of the observed phenomena. In practice, moreover, theoretical work will significantly reduce the experimental effort required by screening many possibilities and guiding new experiments. Since this will have (and already is having) a major technological impact, increased attention is being paid to simulation of materials by scientific and industrial communities around the world.

4.2.3. Competition and the International Situation

Many of the above procedures originated from research in Europe or at least were developed significantly by researchers within the countries of the EU. The most notable recent example is the DFT-MD approach introduced by R. Car and M. Parrinello. Also, in the field of statistical mechanics simulations (coarse-grained models), European researchers are leading or are among the leading groups. There are many national and international activities which clearly demonstrate the competitiveness of European theoretical materials science. One indicator of this is the many invited talks European theoreticians are asked to give at international conferences. At the same time, there are significant efforts being made in the U.S., partly as a result of the hiring policies of top U.S. universities, partly within projects sponsored by the National Science Foundation (NSF) and other funding agencies. Top materials science departments (for example, at MIT, Stanford, UC Santa Barbara, UC Berkeley, and the University of Minnesota) are currently increasing their theoretical research programmes. All these activities are characterized by their close links among basic experiments, theoretical/numerical investigations and application-oriented approaches. Similar acitivities can be found within the Ministry of the Economy, Trade and Industry (METI, the successor of MITI) projects of the Japanese government. The most notable of these is the project currently headed by Prof. M. Doi, in which scientists from industry and university work at the same location on simulations of macromolecules. It is worth pointing out that many of the theoretical models and methods being used there originated from Europe!

Competition is increasing as theoretical and simulation methods come closer to being directly applied in industry. This means that technology transfer from academic to industry has to be improved, which also requires input from industry beyond the current level! In addition, the significant number of highly educated and motivated researchers at all levels of their careers leaving Europe to go elsewhere has to be recognized as the chief threat to sustained progress in the materials modelling field in Europe. Young PhD graduates are being vigorously sought by the U.S., where they enjoy significantly better job opportunities and salaries. In other words, international competition has to be met on many different levels.

General Reviews

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4.3. Theory, Simulation and Design of Advanced Ceramics and Composites

C. A. J. Fisher | Japan Fine Ceramics, Nagoya, Japan

For most of its history, ceramic science has been empirically based, due both to the application-driven nature of its subject matter and the relative complexity and variety of materials and phenomena it encompasses. One of the striking features of the last twenty years, however, has been the advances made in the field of ceramics theory and simulation, so that in many cases it is now possible to replicate and/or predict the properties of ceramics "in silico". This has been facilitated by the astounding growth in computing power over the last two decades, in conjunction with the refinement and expansion of simulation algorithms. Computers combine the best aspects of mechanical models (viz. enhanced visualization and manipulation) with the ability to process vast amount of data, and are therefore excellent tools for testing our understanding of the complex nature of advanced ceramics and composites, often providing new insights.

Ceramic science forms only one part of the study of materials, itself a highly multidisciplinary field relying on and utilizing concepts from solid state physics, chemistry, solid mechanics, rheology, and engineering, and so on. It is no surprise, therefore, that many aspects of ceramics theory and simulation borrow from and build upon knowledge gained from other fields, especially those dealing with metals and polymers. In this section we focus upon those aspects of modern materials theory peculiar to ceramics, and present an outline of the current status of ceramics research, its future needs and priorities.

4.3.1. State of the Art

Fig. 4.4 summarizes the main techniques currently used to model ceramics, and roughly indicates the time and length scales to which they apply. The scope of each of the modelling regimes is constantly being expanded as computational resources are pushed to their limits. We can therefore expect greater overlap between the phenomena and length/time scales handled by different techniques, making it possible to develop reliable multi-scale modelling techniques (see Sect. 4.3.2).

(a) *Ab initio* and atomistic modelling

The methods used to model ceramics on the atomic scale are essentially the same as those for simulating metals. At the most detailed level, *ab initio* quantum mechanical (QM) calculations take into account the electronic structure by solving, at some level of approximation, the Schrödinger equation. Despite the remarkable array of techniques available, calculations are typically performed within one of two computational frameworks. Hartree-Fock (HF) theory is the older of the two, and describes the system in terms of atomic orbitals, with the many-body wave function approximated as the product of one-electron wave functions. The second approach is based on Density Functional Theory (DFT) – usually within either the Local Density Approximation (LDA) or Generalised Gradient Approximation (GGA) – in which the energy of the system is a function of its total electron density. DFT is computationally easier to apply to solid state systems, and so will become increasingly important in the study of ceramics over the next few years. This perception is reflected in the award of the 1998 Nobel prize for Chemistry to Walter Kohn of the University of California at Santa Barbara, the father of modern DFT.

Several academic and commercial software packages are available for performing QM calculations, some of the better known being CRYSTAL, GAUSSIAN, CASTEP and DV-Xα. However, these methods are all computationally expensive; even with today's computers, calculations are confined to at most a hundred or so atoms. Since many ceramics have large unit cells, this places limits on the range of structures and phenomena to which these methods can be usefully applied. Nevertheless, these methods are vital for the accurate determination of the fundamental physics and chemistry of ceramics, and are already being used by industry to solve problems where knowledge of electronic structure is important, e.g. molecule-surface adsorption during catalysis.

The more general approach to atomistic modelling is to derive "effective" interatomic potentials (sometimes referred to as "force fields"), that describe the variation in energy between atoms in analytical or numerical form. Atoms are treated as rigid particles (i.e. the motion of individual electrons is ignored), although the "shell model" can be used to take into account electronic polarization. Using these potentials, of which there is a wide variety ranging in sophistication from the simple two-body Lennard-Jones type to multi-body Embedded Atom Method (EAM) potentials, much larger systems can be studied – up to a

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million atoms on today's supercomputers. More commonly, simulations are performed with empirical potentials on workstations and the latest PC's for a thousand to tens of thousands of particles.

The chief difference between atomistic simulations of ceramics and other substances is the need to take into account the long-range Coulombic interactions between charged particles, as many ceramics are at least partially ionically-bonded. The Coloumb energy, which falls off as 1/distance, is traditionally handled by the Ewald method, although other methods, e.g. the Fast Multiple Method (FMM), are increasingly being used in an attempt to reduce the amount of computational time spent in this critical part of the simulation.

Once an atomic interaction model has been selected, essentially the same techniques for simulating metallic and polymeric systems can be applied to oxides, nitrides, carbides and other ceramics (see Fig. 4.4). These methods are now used routinely to predict the properties of perfect crystals, bond states, defects, surfaces and grain boundaries, covering phenomena such as surface catalysis, solution energies, atomic diffusion, wetting, friction, crack growth and phase changes. The chief challenge for atomistic modelling over the next decade will be to develop reliable interatomic potentials that are transferable between different compounds and coordination environments. This has motivated the development of semi-empirical methods, such as the Tight Binding (TB) method, which, although more time consuming than fully empirical methods, provide increased accuracy and are appropriate for a wider range of bonding environments. Another major challenge will be to overcome the short length and time scales to which atomistic simulations are currently limited, particularly in the case of dynamic simulations, so that a wider range of phenomena, such as "normal" (non-rapid) ionic diffusion in crystals, can be simulated.

(b) Meso-scale modelling

Most ceramics are used in polycrystalline form, and it has long been recognized that a ceramic's microstructure has a profound influence on its properties, including appearance, strength and corrosion resistance. A major goal of current research is therefore to develop, based on both established and yet-to-be-developed theories of sintering and grain growth, simulation methods that can reliably reproduce the time-evolution of microstructures. Computer simulation allows the simultaneous solution of large numbers of non-linear equations, and therefore provides a means to consider several mechanisms in the same model. However, apart from a few examples, computer simulations still can not routinely and reliably describe the behaviour of real materials due to simplifications necessary to make the calculations tractable. Nevertheless, many simplified models have provided a sound basis for understanding the basic mechanisms involved in microstructural

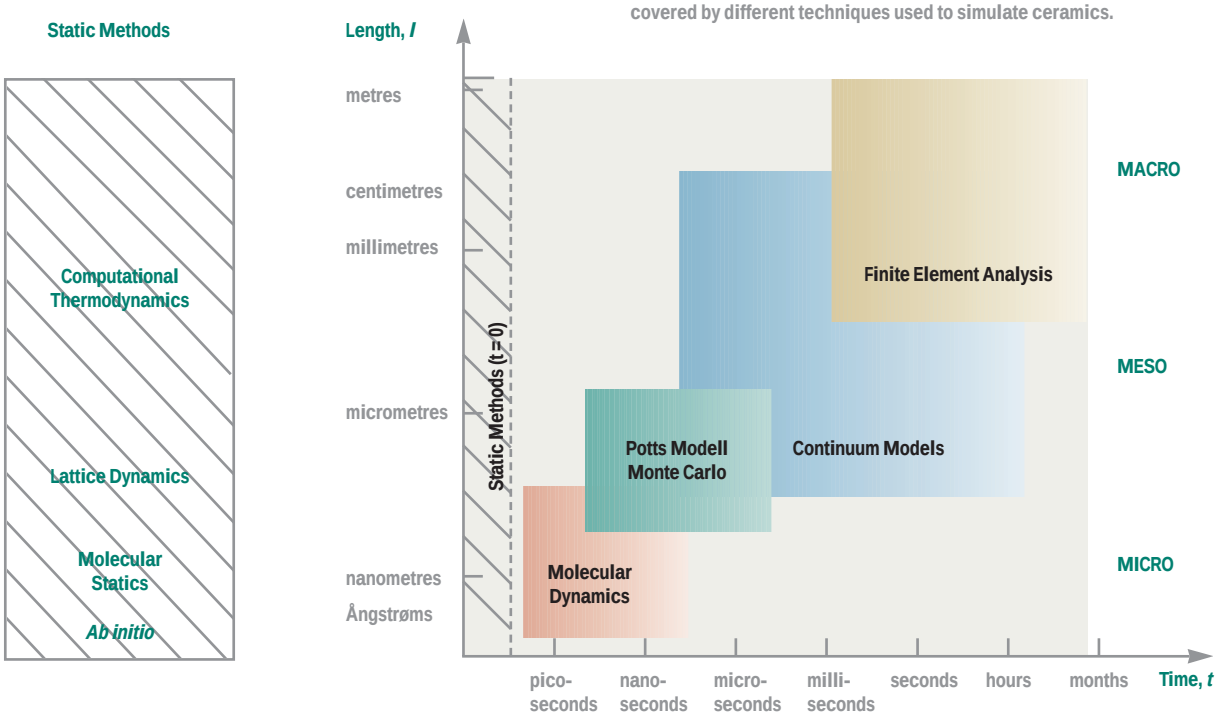

Fig. 4.4. A schematic representation of the time and length scales covered by different techniques used to simulate ceramics.

development, and are an important step in the formulation of more sophisticated general theories.

Most techniques for modelling the meso-scale are continuum methods. These have been used to describe a vast range of phenomena from ceramic processing (extrusion, pressing, slip-casting, thermal spraying, etc), sintering, Zener pinning and Ostwald ripening, to ferroelectric domain switching in magnetic ceramics and crack-bridging in composites. They are usually based on principles such as constitutive theory and balance laws from solid mechanics, thermodynamics or the Cahn-Hilliard and Ginzburg-Landau equations. Common techniques from other fields are now also being successfully applied to ceramics, e.g. the Cellular Automaton method and Population Balance modelling.

Unlike continuum techniques, the Potts Model Monte Carlo method does not rely on explicit input of thermodynamic and kinetic characteristics into the model. The "ceramic" is represented on a square or triangular lattice as an agglomerate of particles with different interface energies, and statistical sampling is performed to find configurations of increasingly lower energy. Methods have been developed for treating grain growth and crack propagation in multi-phase systems, as well as complicated phenomena such as liquid phase sintering, an important process in the formation of many ceramics. 2D simulations can often reproduce the chief characteristics of microstructural evolution of ceramics, while 3D models are often necessary, despite the large increase in computational costs they entail, for quantitative agreement with actual materials. The primary limitation of this method is in deciding on the range and relative size of the interface energies, although this may be overcome in the future by using multi-scale modelling techniques.

(c) Macro-scale modelling

Many macro-scale processes, such as those involved in the formation and use of ceramic components, have been successfully modelled using Finite Element Methods (FEM). This is one of the earliest techniques applied to materials modelling, and is used throughout industry today. Many powerful commercial software packages are available for calculating 2D and 3D thermomechanical, electromechanical and optical properties/processes (e.g. indentation response, densification, and piezoelectric effects). Recent developments in Continuum Damage Mechanics (CDM) theory allow FEM to be used to treat fracture, crack growth and related phenomena. FEM is the simulation method closest to real ceramic applications, usually relying on a large database of measured materials properties as input.

Another successfully applied field of "macro-scale" modelling is computational thermodynamics. Software packages such as Thermo-Calc, Chemsage and Fact use the laws of thermodynamics and large databases of thermodynamic data to predict phase diagrams and the chemical stability of single, binary and multiple phase ceramic systems at various temperatures and pressures. This field also includes the rapidly advancing field of first-principles and statistical thermodynamics calculations of inorganic materials. Computational thermodynamics thus has the unique position of being applicable to all length scales. Unfortunately the influence of metastable phases, kinetic effects and non-equilibrium conditions, which strongly affect the microstructure and properties of ceramics, cannot yet be handled adequately. Such methods are currently being developed for metallic systems, so it is reasonable to assume that ceramic scientists will extend their use to ceramic materials in the near future.

4.3.2 Future Research Goals and Priorities

The interplay between theory, modelling, experiment and final application of ceramics is illustrated in Fig. 4.5. The ultimate goal is to reduce the dependence on experiment and empirical measurement, and perform at least the preliminary stages of materials selection and design on computer. From an industrial viewpoint, the aim is to reduce both the cost and time of developing materials for new applications, or to replace materials in current applications with new, improved ones, for reasons of cost, performance and/or environmental compatibility. In pursuit of this target, the following trends and priorities for ceramics-related simulation have been identified.

(a) Ceramics theory

Nowadays theory and simulation are often closely interrelated, with one serving to confirm and/or modify the other in a symbiotic fashion. As experimental techniques become more precise, with many devices now capable of manipulating structure on the atomic level, our ability to compare theoretical predictions directly with experiment via computer simulation is increasing. There is no doubt that novel phenomena in advanced ceramics await to be discovered – and also explained – well into the future. Indeed, adequate theoretical explanations for some phenomena, such as superconductivity in cuprate ceramics and the varistor effect in zinc oxide ceramics, are still being sought. Other underlying theories used in ceramics simulation are on the whole well established, e.g. quantum mechanics, thermodynamics, fracture mechanics and

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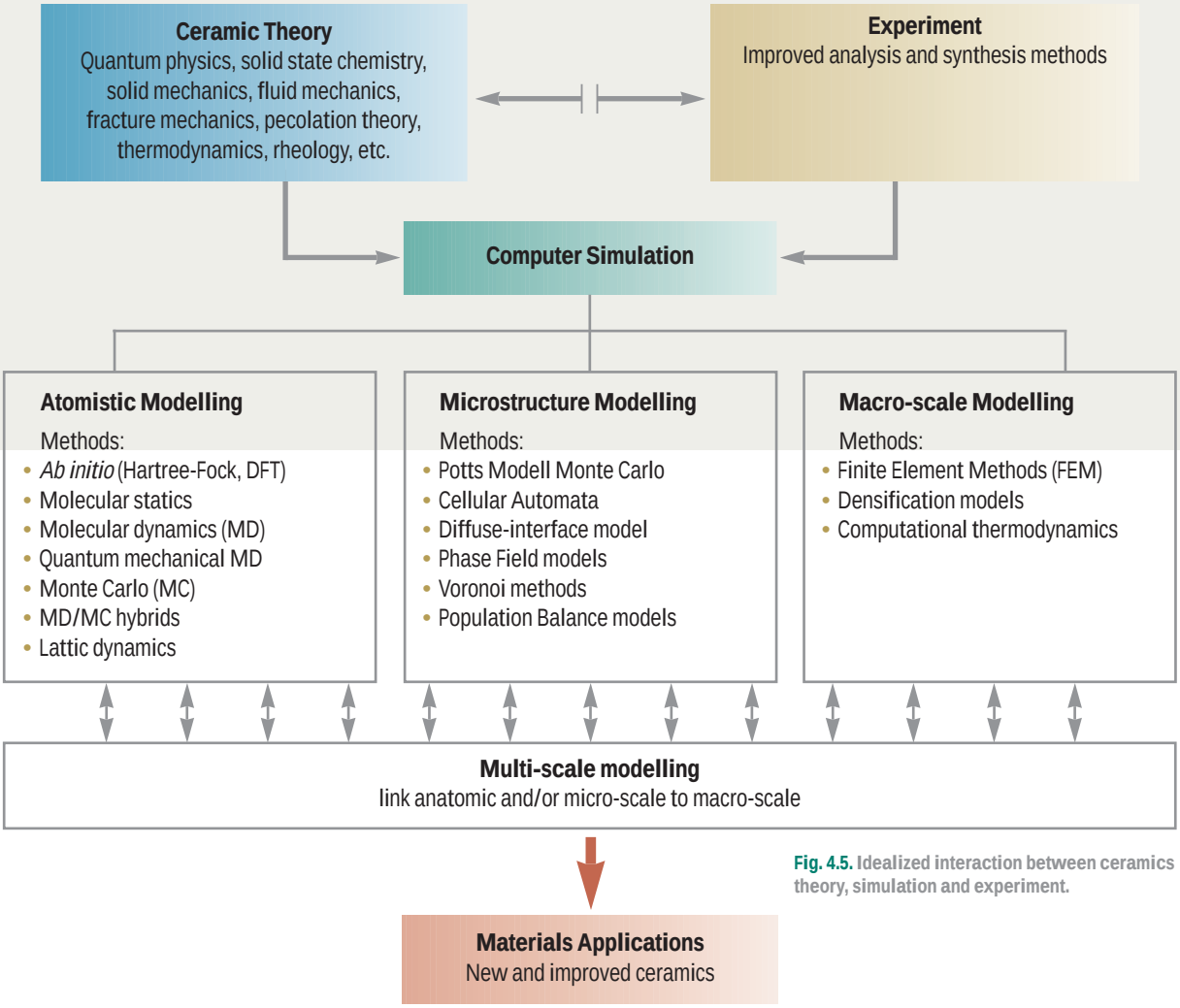

Fig. 4.5. Idealized interaction between ceramics theory, simulation and experiment.

dislocation dynamics. Challenges arise in applying and extending these to the structural and/or compositional complexities typical of advanced ceramics and composites. The brittle nature of these materials means that their physical properties are often controlled as much by their macro-scale and microstructural conformation as by their chemistry. More comprehensive and "holistic" theories of microstructural evolution over short and long time periods need to be developed if the properties of ceramics are to be properly understood, controlled and improved.

(b) Multi-scale modelling

Fig. 4.6 lists several short-term and long-term priorities for research into simulation techniques for given length scales. Although these are very important for understanding certain phenomena within specific fields, from the point of view of overall materials design, the development of methods for performing "multi-scale" or "hierarchical" modelling is perhaps the most pressing need.

"Multi-scale" modelling is the combination of various techniques that treat disparate length (and time) scales into a single consistent simulation. The simplest approach is to use output from small-scale simulations as the input to larger scale calculations, the so-called "bottom up" approach. Other strategies incorporate feedback loops, or perform detailed, computationally expensive calculations only at critical points in the simulation. Hurdles that need to be cleared include deciding where the transition from "discrete" to "continuum" behaviour occurs, and how representative small-scale simulations are of large-scale phenomena.

The concept of multi-scale modelling has been applied to simulation of metals for several years now, but it is only just beginning to be pursued by modellers of ceramics. Two recent examples include atomistic simulation of crack fronts combined with continuum treatments for the surrounding matter, and Potts Model Monte Carlo simulation of microstructure in combination with stress-strain

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and temperature distributions from FEM. Successful development of these methods will undoubtedly require large investments of money, brain and computing power. However, in terms of the reduction in use of raw materials, improved properties and performance, and reduced product development time for advanced ceramics and composites, the rewards will be substantial.

(c) Synthesis and processing of ceramics

The fundamental nature of sintering and grain growth and its influence on the properties of ceramics, particularly for engineering and structural applications, means that reliable simulation techniques will be in great demand in the years ahead. Atomistic, microstructural and macro-scale simulations all have a part to play in elucidating the mechanisms involved. Only a multi-scale model, however, will be able to handle the interactions between different microstructural components and macroscopic conditions, and it is difficult to envisage any other means of reliably predicting the microstructures of actual ceramics solely within the computer. A great deal more research, both theoretical and practical, needs to be done before such techniques are realized.

The increasing importance of chemical methods for synthesizing advanced ceramics, particularly solution-based processing and gas phase methods (e.g. chemical vapour deposition), means that increased attention should be paid to modelling these systems as well. Analytical models, including FEM and fluid dynamics, have been used to study such processes, but more work remains to be done on simulating processes such as pyrolysis, crystal growth and gas phase reactions from the atomic and nano-levels.

(d) Smart materials

Irrespective of whether a material is intended for functional or structural use, simulation methods are available (albeit with different levels of accuracy) for investigating its physical, chemical, electronic and mechanical behaviour. Indeed, the growing field of smart materials, in which both functionality (e.g. sensing) and structural integrity (e.g. strength or durability) are combined in the same ceramic or composite, will greatly benefit from the use of computer modelling for this very reason. Models that can take into account multiple factors such as grain size, diffusion rates, external pressure levels, and so on, will allow the behaviour of smart materials to be predicted and optimized faster than would otherwise be possible by trial-and-error experimentation.

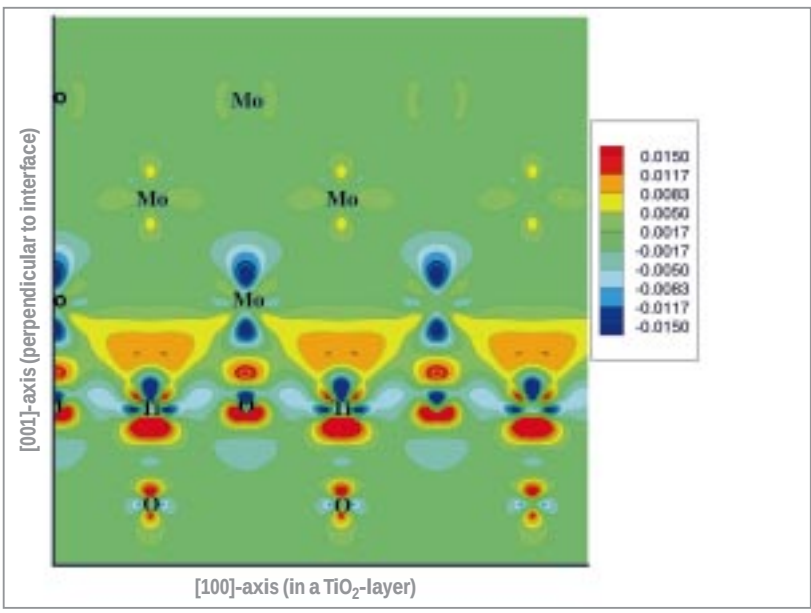
(e) Nanoceramics

As part of the nanotechnology drive of the late 1990s, work commenced on the development of nanoceramics, with their promise of superior properties and possibly even new phenomena. Because of the length scales involved, atomistic and microstructural simulation techniques naturally lend themselves to the study of these materials. Combined with advances in high-resolution instrumentation (for calibration and validation of simulation/theory) and processing (for manipulating ceramics at the nano-scale), these simulation techniques will become essential tools in the study and design of nanoceramics. As components (e.g. crystal grains) become smaller, the relative proportion and importance of interfaces increases, so that the use of simulation techniques to understand interface structure and behaviour will be a central part of nanoceramics research.

(f) Interface science

Not only in nanoceramics, but also in most polycrystalline materials and especially composites, interfaces play an important, often crucial (e.g. zinc oxide varistors) role in determining a material's properties and performance. A major goal of materials research over the next few years will therefore be the simulation and eventual design of interfaces, inlcuding grain boundaries and surfaces.

Bonding of ceramics to other materials, e.g. ceramic coatings, is an important technological issue that will require substantial research and innovation. New methods for modelling interfaces in heterogeneous and/or multi-material systems (e.g. ceramic-polymer and metal-ceramic interfaces) need to be developed, since the fundamental



Mo/$SrTiO_3$ (001) contact: local density functional theory (*ab initio* mixed-basis pseudopotential calculations): electron density difference between interface and free surface, showing Mo-O nearest-neighbour bonds and Mo-Ti next-nearest neighbour bonds across the interface (Th. Classen and Ch. Elsässer, MPI für Metallforschung Stuttgart).

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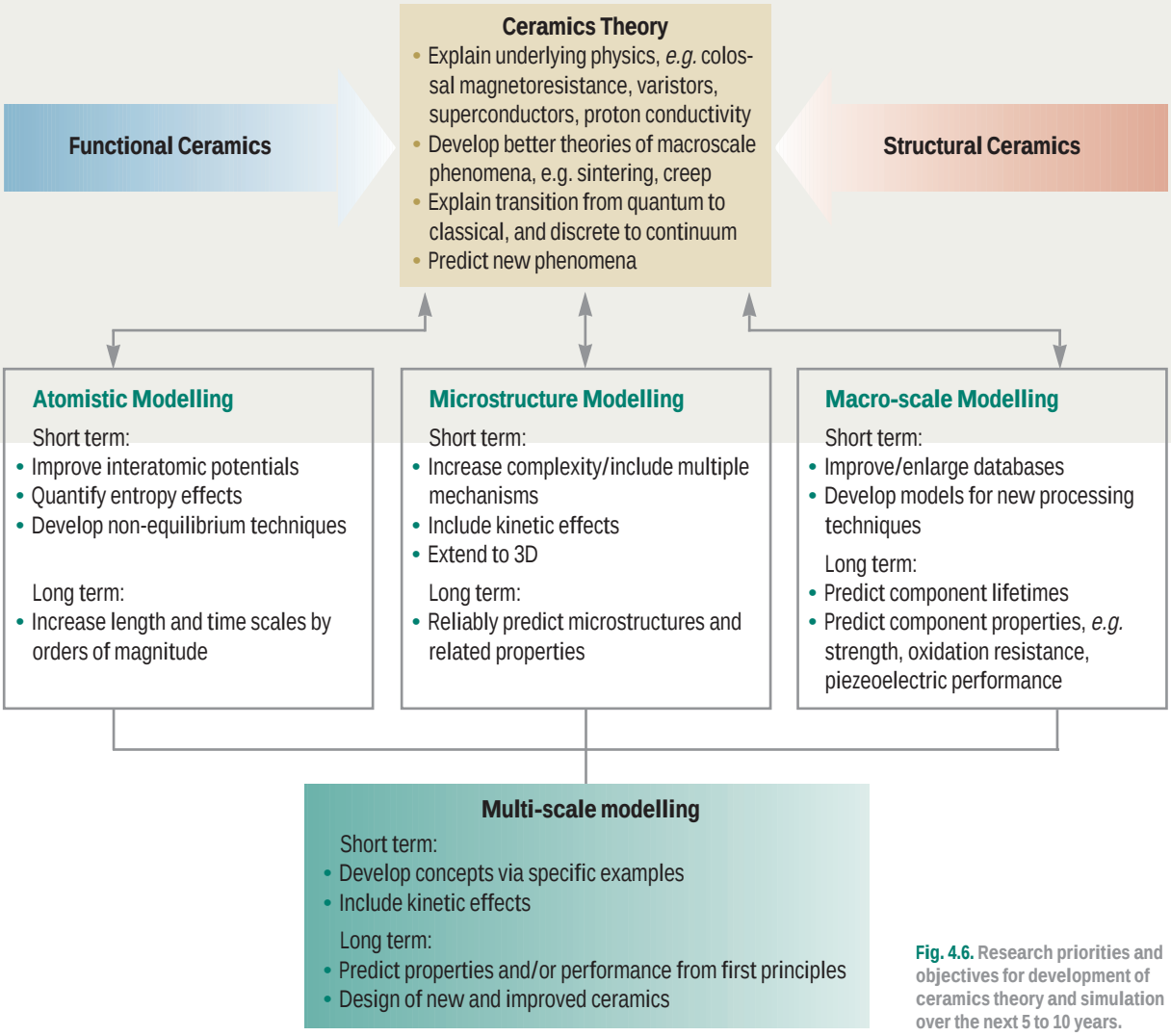

Fig. 4.6. Research priorities and objectives for development of ceramics theory and simulation over the next 5 to 10 years.

differences in bonding, structure and symmetry between different phases make them difficult to simulate with current methods. In addition, the virtually infinite number of permutations of interface orientations, segregation effects, strain and defect states in real materials needs to be taken into account. Assuming that time- and length-scale limitations can be overcome (e.g. using new methods such as hyperdynamics, parallel replica dynamics or temperature-accelerated dynamics), atomistic simulations will become important sources of data about the structure and properties of ceramic interfaces. For macro-scale components with nano-level organization, one possible scenario is that results of atomistic methods are used to test and/or develop general principles, and these scaled up for larger simulations via some multi-scale modelling schema.

(g) Design of ceramics

Despite active research and significant progress over the last decade, materials modelling has yet to have a significant impact on the design of advanced ceramics. This is perhaps not surprising given the newness of the field and the small numbers of researchers in it. Generally speaking, given the time it currently takes to develop, validate, perform and interpret computer simulations, it is still often faster to run a large series of experiments on different materials and pick the best one. To overcome this "time-lag", and exploit the potential of computer modelling to streamline and improve the design process, more robust simulation techniques and software will need to be tried and tested over the next decade, with input from industry and software companies. This process is expected to occur faster for ceramics used in functional applications, such as sensors and electronic components, where miniaturization and improved synthesis methods provide greater control over a material's composition, structure and behaviour, than for structural ceramics, where the number of controllable and uncontrollable variables is greater.

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One example of the potential of computer modelling to revolutionize materials design is a recent report in Nature of the use of computer simulations to predict the existence of an ultra-hard phase of TiO_2. This new phase was subsequently synthesized, and found to have properties close to those predicted. It should also be pointed that in certain areas where the materials problem is well defined, such as use of zeolite catalysts and molecular sieves in the petrochemical industry, computer simulation has been making useful contributions to materials design for some time.

Between the extremes of "molecular design" and "component design" lies the field of microstructural design. Although likely to take longer to develop, tools for simulating ceramics microstructures will have an enormous impact on the design of ceramics, resulting in improved strength, toughness, high temperature stability, thermal conductivity, etc, and largely replacing the "trial-and-error" methods used today. Depending on how rapidly multi-scale modelling techniques can be realised, the computational design of ceramics and composites from the nano- and micro-levels to the final component should be feasible within the next ten to fifteen years.

4.3.3. Research Infrastructure

Compared to metals, polymers and "biotech" materials, the number of researchers modelling ceramics is relatively small. This imbalance needs to be addressed by support for both basic research into advanced ceramics as well as their high-tech application. Similarly, many of the problems currently encountered in ceramics theory will only likely be solved by combined contributions from researchers in different fields. It is therefore important to promote interdisciplinary collaboration, particularly between physicists, chemists, materials engineers and computer scientists. Students should also be encouraged to learn both experimental and simulation techniques for studying advanced ceramics and composites.

To remain at the forefront of materials simulation, European laboratories will need access to increasingly faster and more powerful computers. The cheapness and ubiquity of personal computers (PCs) means that an economic way of constructing a parallel processing system for handling large-scale simulations is to connect several PCs in a simple array network. There is still a need for access to supercomputing facilities, however, for large research and collaborative efforts, particularly in the case of atomistic/quantum mechanical calculations. For example, ultra-large-scale (supra-million atoms) simulations for investigating phenomena on the micron level will require massively parallel architectures to be performed in a reasonable time frame.

Europe is in an excellent position to take advantage of advances in computer modelling of ceramics and composites because of its core of top-class theoretical researchers and its tradition of innovative thinking in the physical sciences. Research teams from the UK and Germany, as well as many from Italy, France, Switzerland, The Netherlands and elsewhere, lead the way in many areas of ceramics theory and modelling. Fostering of researchers, theoreticians and experimentalists within the European framework, as well as internationally, should therefore be given high priority to ensure continued progress in this field and also to give European industries the competitive edge they need in an increasingly high-tech world.

4.4. Modelling Strategies for Nano- and Biomaterials

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The science and technology of materials have often been said to set the milestones of human progress. Indeed, important stages in the history of civilization are often referred to as the Stone Age, Bronze Age and Iron Age. As we enter the first decade of the 21st century, we can look back on the tremendous impact and benefit materials technology has had on human life. At the same time, we are entering one of the most exciting eras in terms of accelerating technological innovation in the history of mankind. There are unprecedented opportunities for improvements in health and standards of living for humanity as a whole. The interdisciplinary boundaries between materials science and biology, physics, and chemistry will provide fertile ground for establishing a new knowledge base for emerg-

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ing nano- and biomaterials technologies. These research areas, while providing tremendous opportunities for scientific discoveries and technological innovations, demand intensified efforts to develop new theories and modelling strategies for complex materials systems.

The main purpose of this article will be to show that materials theory has been a basis and guide for the development and improvement of new generations of materials in the aerospace, automotive and microelectronic industries. There is no reason to suspect that theory will play any lesser role in the emerging nano- and biomaterials fields. In fact, we strongly believe that theory will play a more important role because the complexity of the systems used in these new areas can only be overcome by combining experimentation with effective modelling. We strongly recommend that modelling and simulation be included as essential parts of all present and future European programmes on materials research.

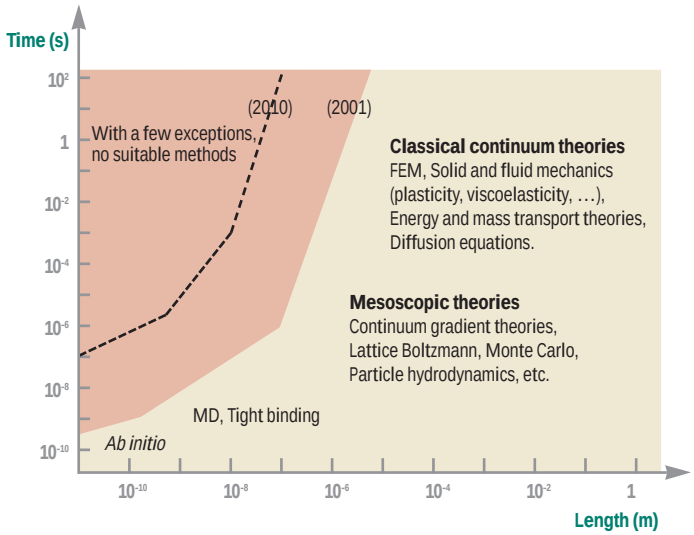
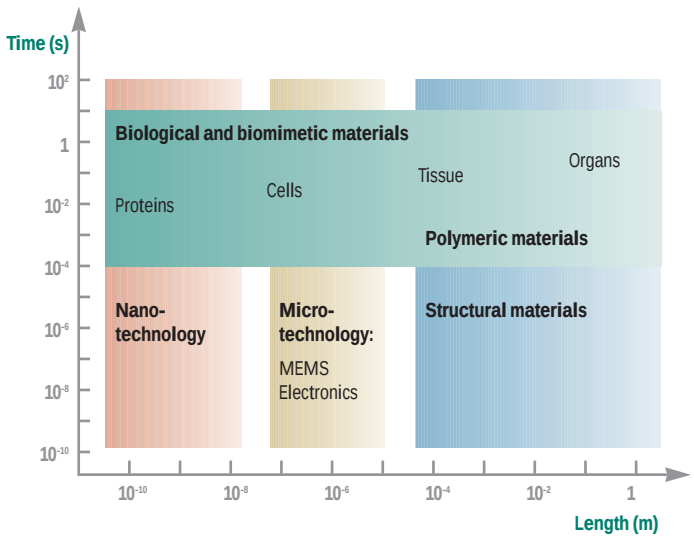


Fig. 4.7. The state of the art and present frontiers of theoretical methods in materials modelling in terms of length and time scales of applicability. The yellow region represents problem areas where methods have been developed and the orange region represents areas where no suitable methods presently exist. The dotted line is the projected frontier by 2010.



Modelling has played an indispensable role in the development and improvement of new materials for industrial, military and civilian applications. The past two centuries have witnessed tremendous progress in our understanding of metals. The field of metallurgy has evolved from an art to a scientific discipline firmly based on the theories of dislocation, creep, fatigue and plasticity. Tremendous progress has also been made in our understanding of ceramics, glass, semiconductor, and polymer materials. On the other hand, our understanding of nano- and biomaterials such as quantum dots, nanostructures, molecular assembly, proteins and DNA molecules, is still at a very primitive stage. Similarly, while synthesis and processing of many structural materials has reached a state of maturity, there is a general lack of theoretical understanding on nano- and bio-synthesis methods including thin film growth and processing, nanofabrication, biomimicry and self-organization. This is due to the complexity of these processes and insufficient understanding of the underlying physical principles.

Classical methods in materials theory include solid mechanics, fluid mechanics, the finite element method (FEM), diffusion theories, thermodynamics, and statistical mechanics. One can hardly think of any industrial applications where at least one of these theories has not played a crucial role in its development. The theories of solid and fluid mechanics, including structural mechanics, strength of materials, plasticity, fracture, and aerodynamics, have guided the development of new materials and new design methods now widely used in the aerospace, civil engineering, automotive, nuclear and computer industries. Quantum electronic theories have formed the basis of device physics in microelectronic and optoelectronic industries. While the theories of dislocations, plasticity, fracture and creep have guided the development of materials such as superalloys, polymer composites and ceramic composites, quantum simulation techniques have now been introduced to investigate and/or design molecular materials such as nanotubes, proteins and new pharmaceutical drugs. Modelling and simulation techniques affect all stages in the development and improvement of new materials, from the initial formation of concepts to

Fig. 4.8. Typical length and time scales for a number of technological areas where materials modelling and simulation are essential. By overlaying this plot on Fig. 4.7, it can be seen that there are presently no suitable methods to treat much of the nano- and biomaterials technology within realistic length and time scales.

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synthesis, characterization and properties. For example, the FEM method is widely used to evaluate design concepts, to optimize testing and fabrication methods, and to link structural and functional performance to microstructure of materials.

Recent decades have also witnessed tremendous progress in quantum and atomistic simulation methods such as DFT. An overview of the state of the art of such methods has already been discussed in Sect. 4.2. Quantum simulations are now being used to study the behaviour of nanostructures such as carbon nanotubes and a myriad of biological molecules such as various types of proteins, membrane lipids and vitamins. These simulation methods are not only limited by the number of degrees of freedom but, more importantly, also by the time scale. Typically, *ab initio* quantum methods are applied to system sizes of a few hundred atoms and time scales up to a few picoseconds. In comparison, classical molecular dynamics methods are based on direct time integration of Newton's laws of motion and can now treat systems of up to one billion atoms with time scales on the order of nanoseconds. These restrictions often limit the application of quantum methods to the study of nano- and biomaterials. One possible remedy to this problem is to develop mesoscale theories to bridge the *ab initio* quantum concepts and continuum methods. Present examples of such mesoscale theories are continuum gradient theories, Boltzmann transport theories, Monte Carlo methods, and particle hydrodynamics methods. Another promising approach is Voter's time or temperature accelerated molecular dynamics methods. Advances in computing power in the next decade will significantly expand the regime of applicability for many of these methods.

Based on past experience, it should be possible to extend the time scales of quantum and atomistic methods by one or two orders of magnitude by 2010.

4.4.1. State of the Art and Present Frontiers

Fig. 4.7 shows a schematic representation of the current state of the art of materials theories with respect to both length and time scales. Typically, classical continuum theories are phenomenological theories based on fundamental physical principles requiring empirical parameters determined from experiments. As such they are often limited to large length scales (above 1 µm) with few time scale limitations. In contrast, *ab initio* quantum methods have in principle no empirical parameters, hence requiring no fitting with experimental data. Such methods should in principle be able to predict experimental outcomes, and hence be extremely powerful. Their main limitations are the short time scale and computational expense, which often prevent them being directly applied to real engineering problems. In between the *ab initio* and classical methods are a host of mesoscale methods that have been developed to bridge the gap between quantum and continuum methods. With a few exceptions (for example, elasticity theory), there are usually no suitable methods to treat problems with system sizes on the order of microns and time scales spanning microseconds and above. On the same length-time plot, Fig. 4.8 shows typical length and time scales for a number of areas of technological application. Comparing Fig. 4.7 and 4.8, one sees that while existing theories are most mature for structural material applications, much of the emergent technology areas concerning nano- and biomaterials require new theoretical tools that are not available to date. For example, protein conformation and folding is one of the most important problems in biomaterials. A comprehensive investigation of such problems would require the development of theories that are appropriate for length scales from a few tens of nanometres to one micrometre and above and time scales from microseconds and beyond. Development of methods for these length and time ranges should be achievable by the next generation of theoretical materials scientists and will provide significant economic benefit to society.

4.4.2. Possible Areas of Breakthroughs

Overlaying Fig. 4.8 on Fig. 4.7 reveals that the central issue of computational materials science is to develop new theories applicable to small length scales and large time scales. Such efforts have the potential to lead to revolutionary breakthroughs in materials modelling and should receive the highest priority for research. Also, four possible areas for more breakthroughs that can have a large impact on emergent materials technologies in the coming decade:

(a) New modelling strategies for complex material systems

At present it still seems unlikely that we will be able to treat all of the interesting problems by *ab initio* methods, at least not in the forseeable future. Even if this were to become possible, the analysis of the enormous amounts of data generated from computer simulations would itself require massive computing power and a comprehensive modelling strategy. Therefore, we need to consider modelling strategies for complex material systems. Such modelling strategies should focus on the multi-scale and multi-physics nature of emergent problem areas in materials

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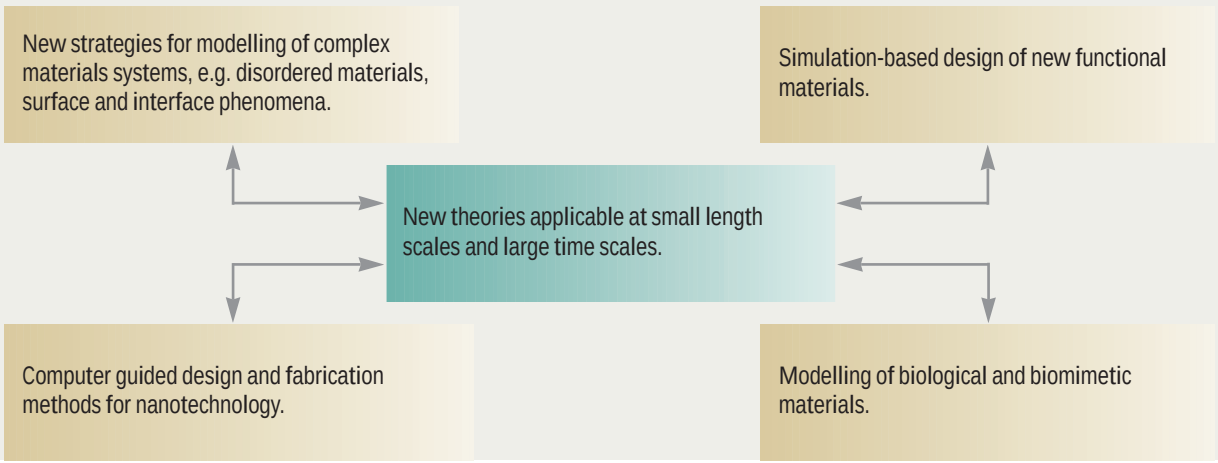
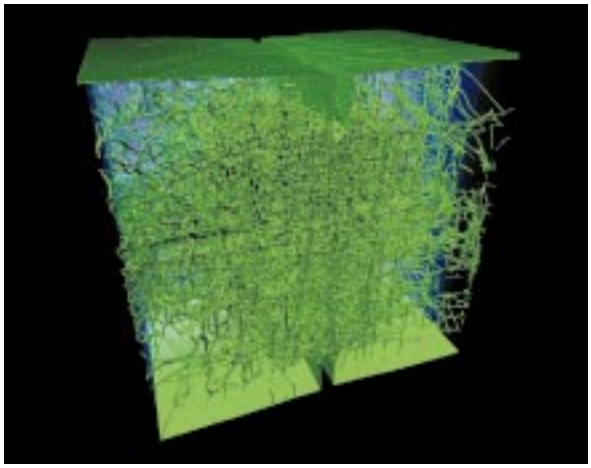


Fig. 4.9. The priority research areas for materials theory. The central block represents the core activity that should lead to revolutionary breakthroughs in theories and methods applicable to problems with small length and large time scales. The four surrounding blocks represent more evolutionary paths that can nevertheless have a large impact on emergent materials technologies.

science. An example might be disordered materials such as polymeric materials where quantum chemistry methods must be used together with atomistic simulations and finite element methods to model phenomena ranging from electronic structure to molecular structures to polymer domains to macromolecular conformation and the macroscale continuum.

(b) Simulation-based design of new functional materials

New integrative methods that bridge modelling at the material level (e.g., composition, structure, morphology) to the functional level (e.g., quantum dots, conducting or semiconducting nanotubes, enzymes) will revolutionize the way that new materials are discovered and developed. New methods for small length and large time scales will be especially important for this development. An example would be the design of molecular electronic devices for future information technology (Fig. 4.9).



Snapshots of 1-billion-atom molecular dynamics simulations of work hardening in a copper single crystal (F. Abraham, H. Gao and coworkers): Dislocations are nucleated at two pre-exisiting cracks. The resulting plastic flow has significantly blunted the crack tips.

(c) Computer guided methods for nanotechnology

Predictive methods to guide nanofabrication will be required for the nascent nanotechnology industry. These methods must be firmly based on physics and have the capability of simulating the nanofabrication process under realistic conditions. One example is the use of kinetic Monte Carlo methods together with *ab initio* methods to model deposition and self-organization of nano-grained magnetic media for the next generation of information storage devices. In such a scheme, information from *ab initio* calculations at the unit cell level is passed to a Monte Carlo algorithm via an event catalogue to simulate the self-organized atomic deposition process.

(d) Modelling of biological and biomimetic materials

Materials scientists have the opportunity to make significant contributions to the development of biological materials for both medical and engineering applications. For example, one of the emerging areas of research is tissue engineering where physics and engineering principles are applied to guide the differentiation of biological stem cells to form specified tissue or organs for medical applications. Questions of how cells interact with patterned or unpatterned metal, ceramics and polymer substrates are important for the development of bio-compatible and biodegradable scaffolds. There are tremendous economic benefits to be realized and, at the same time, many important scientific questions. Conversely, in the field of biomimetic materials one tries to learn from biology the basic principles used by natural evolution to construct materials with superior properties such as adhesion, hardness, and mechanical strength. For example, naturally

occurring materials such as sea shells are made of nanocomposites consisting of alternating layers of minerals and proteins. Such composites exhibit mechanical strengths which are orders of magnitude higher than the constituent phases alone. The mechanisms by which such high strength is achieved are still not well understood. By multiscale modelling and simulation, we hope to learn the basic principles of biological materials and achieve similar materials design in the laboratory through micro- and nano-fabrication methods.

In each of the above examples, modelling plays a crucial role in hypothesizing and formulating basic principles and guiding the development of new materials.

4.4.3. Strategic Alignment of Europe with respect to the U.S. and Japan

With the rapid globalization of the world economy, Europe is facing increasing competition from the U.S. and Japan. The U.S. is heavily investing in nano- and bio-technologies, as reflected by the fact that the funding for the U.S. National Institute of Health has quadrupled over the last 5-10 years and this trend is increasing at an exponential rate. At the same time, the National Science Foundation (NSF) has officially recognized nanoscale modelling and simulation as the major pillar of nanotechnology and is in the process of implementing a series of new initiatives on nanoscale materials modelling. Biomedical engineering departments are being founded at all major U.S. universities (MIT, Stanford, Columbia, Johns Hopkins, Georgia Tech, etc) and are strategically oriented to becoming the major research direction in the 21st century. There is a dramatic increase in the number of students enrolling in life science courses. For example, more than 50% of the undergraduate students at Stanford University declare their major to be related to the life sciences. It is estimated that there will be about 200 new faculty positions in the U.S. in the field of bio-engineering within the next 3 years. Japan is also leading in several key areas of micro- and nanotechnology, especially in the areas of optoelectronics and nanoelectronics. As these technologies are essential for its economic well-being, Europe simply cannot afford to yield the competitive edge to the U.S. and Japan and must take immediate action to establish and maintain a sound scientific base for these newly emerging technologies.

4.4.4. Conclusions

There are enormous new opportunities for research in materials theory in the areas of nano- and biomaterials technology. New theories or methods for applications with small length and large time scales are likely to lead to revolutionary breakthroughs. In addition, we recommend four modelling areas that have the greatest potential for industrial impact in the next decade. These areas are new modelling strategies for complex materials systems, simulation-based design of new functional materials, computer-guided methods for nanotechnology, and modelling of biological and biomimetic materials.

Conclusions

Theoretical modelling of materials has proven to be a successful and valuable part of the science and engineering of materials. The applicability of materials theory to almost any established and newly emerging topic of materials science (see Fig. 4.2) promises that it will play an increasingly guiding, stimulating and visionary role in the search for novel materials. This observation necessitates increased attention to and funding of theory and modelling within materials research programmes in Europe.

The reason for the success of materials modelling is its ability to quantitatively model and predict the complex structures and properties of real materials. Consequently it will soon be possible to “create” novel materials and devices by theoretical means, ranging from structural design via synthesis routes to functional properties. This predictive power originates from the fact that the microscopic concepts of modern materials theory are grounded on principles of solid state physics and chemistry for describing interactions between nuclei and electrons.

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European researchers in academic and industrial laboratories have contributed considerably to this success in the past, and the European Commission as well as national agencies in the European Union set up funding programmes that made this possible. Now more than ever, a concerted effort is needed to maintain Europe's position (in many cases a position of leadership) at the cutting edge of materials theory and modelling. Without suitable planning and support from government and industry, Europeans will miss out on the economic and social benefits that materials modelling will bring. To avoid such a situation, the following recommendations are made:

- Improved transfer of scientific expertise and computational tools between academic researchers at universities and research laboratories operated by public organisations on the one hand and industrial scientists on the other.

This will allow academics to apply their expertise to important issues and problems in the industrial application of materials, and to educate and train the next generation of students with the skills they need. Industry will benefit from access to the latest ideas and having the materials systems they are interested in being studied sooner. Joint academic/industrial research projects will motivate students to pursue careers in materials modelling because of the challenging and relevant problems they can work on.

- European universities and non-industrial research laboratories are encouraged to establish Materials Theory as a substantial part of their research strategies and promote interaction between theoreticians and experimentalists from different disciplines.

The cross-disciplinary nature of this field can be exploited to stimulate students' interest by including materials modelling components within the curricula of natural science (physics, chemistry and biology) and applied engineering degrees. At the same time, faculty positions for materials theorists will be necessary to provide quality teaching in this field.

With regards to academic research, materials modelling will benefit greatly if traditional distinctions between experimental and theoretical groups can be broken down. For instance, teams of experimentalists and materials theorists working together on the same problem (whether it be fundamental phenomena or device development), with the increased communication and understanding this would bring, should greatly accelerate materials research as a whole.

- European industrial companies should also foster long-term materials theory groups, and provide attractive positions to materials theoreticians who are encouraged to think innovatively and help in the design and development of industrial products.

- European “Materials Modelling Centres” and networks should be established similar to those set up in the U.S. in recent years. These could serve as “intellectual hothouses” for the development and application of computational modelling methods, and house European supercomputer facilities for large collaborative projects.

- The continued expansion of the Internet should also be encouraged, and upgrading of communication networks to the latest technology (e.g. ISDN broadband) should be considered a priority.

The Internet has played an important role in the development of materials modelling by: 1) facilitating rapid communication between researchers, 2) allowing rapid publication of results, and 3) providing connections to remote sites, e.g. for transfer of data to and from supercomputers. Already several software and data repositories exist that are freely accessible by anyone, and their growth should be encouraged.

- Research into faster and more powerful computers should continue.

The backbone of all computer modelling is the hardware it uses. Research into the next generation of computers should therefore be supported. Europe is at the forefront of research into optical and quantum computers, and steps should be taken to ensure that this technology is developed and marketed by European industry. These technologies promise to be orders of magnitude faster than conventional electronic computers, and will revolutionise materials modelling at all levels.

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5. MATERIALS PHENOMENA

Introduction

The science of materials may perhaps be described as the physics and chemistry of materials behaviour, as exhibited by the phenomena observed by subjecting material substances, usually solids, to some action. Time and again new phenomena are discovered. Recent examples involve superplasticity and high T_c superconductivity, which phenomena are also of great potential for practical application.

Materials phenomena are usually classified according to four broad categories: mechanical/physical, thermal, electrical/optical, and magnetic. The boundaries between these categories are by no means fixed or discrete, however, and many interesting and useful phenomena lie at the intersections of two or more categories.

In this chapter the focus is on general aspects of materials behaviour, in contrast with what has been presented in chapters 1 and 2 where the various contributions have been devoted to specific types (classes) of materials. Furthermore, concentration on materials phenomena implies paying attention to fundamental scientific issues. The technology needed to exploit a certain phenomenon does not belong to the core of the discussion here. Yet, various contributions in this chapter depart from a more technological basis. But even then, the discussion should culminate in identification of those materials phenomena that deserve our special interest.

The properties of a substance are intimately related to its structure and the interactions between its building units. Thus, to understand material behaviour it is imperative to know the atomic and electronic structure. Few materials are used solely in their ideal equlibrium state. Non-equlibrium phases can be associated with exceptional phenomena that can make the material amenable to practical applications, e.g., doped semiconductors, or metallic glasses.

It is not at all enough to describe the ideal arrangements of atoms for materials: real materials exhibit properties that are to a large extent determined by non-idealities, as grain boundaries and surfaces and defects in the atomic arrangement. The quantitative description of material properties is very complex, because many length scales have to be considered. Understanding the intrinsic imperfections in the structure of materials and developing models for predicting material properties from atomic to macroscopic scale are cardinal topics of research in materials science.

The basis of any understanding of materials behaviour must be knowledge of the equilibrium constitution: which phases (composition and amount) are present. In principle a description can be provided of the state the system under consideration strives for, including the possible identification of metastable intermediate stages and the net amount of energy gained (or to be delivered). In spite of its long history, important aspects of the theory of material thermodynamics are under development and deserve attention urgently.

Parameters as temperature and atmosphere affect the occurrence and magnitude of a given phenomenon. For example, a strong magnet at room temperature will become an ordinary paramagnetic material if heated above its Curie point,

◀ Transmission polarized light micrograph of a MoO_2 particle (U. Täffner, MPI für Metallforschung Stuttgart)

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and platinum catalysts are rapidly "poisoned" by carbon monoxide gas. Phenomena such as creep, crack propagation and oxidation can be detrimental to materials performance. Hence, what happens to a material once it is in use is an essential aspect of materials science.

The existing theoretical knowledge of the kinetics of material behaviour is very incomplete. There are various reasons for this observation. For example, to couple the driving force (i.e. gain in net energy) directly to a mobility is difficult and a number of important questions can be derived from this conclusion. Further, although many kinetic measurements have been reported for a myriad of systems, a severe lack exists of significant kinetic data obtained from suitable model systems that allow generalization. If we don't improve greatly our understanding of kinetics, there is no chance that we will be able to control the microstructure of materials by means of which the properties of products can be influenced dramatically.

Specific types of materials have not been mentioned until now in this introduction, recognizing the striving for discovery and understanding general, fundamental laws governing materials behaviour. Yet, it goes without saying that certain phenomena are associated with specific material classes and states of matter; see contributions devoted to metals, polymers, colloids, etc. Currently a focal point of interest develops around biomaterials and, for example, the interface between biomaterials and inorganic materials appears a rich source of topics for exciting research.

With a view to the past it can be said that current activities in materials science have been revolutionized by the emergence of small scale systems (e.g. thin films, nanomaterials). The ultimate form of nanotechnology, the handling of single atoms, has become feasible and gives rise to the discovery of new phenomena. Thereby, certain problems in the "classical" areas of research have got an immediate urgency (role of interfaces and surfaces, stress, etc.). It can be seen from the contributions contained in this chapter that this statement is a recurring theme for much of what is presented.

The contributions in this chapter discuss different aspects of materials phenomena, such as thermochemistry, nanoscale effects, electronic, magnetic and mechanical properties. It is not possible to be complete; the items discussed were chosen hoping that the reader will gain an appreciation for the great diversity of the phenomena exhibited by all kinds of materials.

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5.1. Thermochemistry of Materials

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5.1.1. Introduction

The development of new materials is traditionally a very tedious process involving extensive experimental investigations by which composition and processing conditions are varied in a more or less erratic manner until the desired properties are achieved.

The properties of materials depend on phases present, their composition and how they are geometrically arranged in the microstructure involving structural elements on micro, nano and atomic scale. Therefore, a detailed information about temperature and composition stability ranges of the different phases and their transformations and equilibria as well as eventually occurring non-equilibria states are indeed indispensable for a full understanding of the properties and possible applications of a given material. This is true equally for metallic and ceramic alloys as well as for polymer blends.

On the one hand the potential of new engineering materials exceeds by number of possible element combinations all experimental research capacities. On the other hand the already existing data, i.e. the starting base for future research is very huge, scattered, conflicting and increasing by about 20% every year. A considerable amount of resources and time has to go into the evaluation of these data for each project before controlled steps can be set into the "terra incognita" of possibly coexisting phase configurations, microstructures and properties. This increasingly slows down the overall research efficiency.

Reality is that in each of the European countries the intellectual resources, laboratories and people working in this field are sub-critical, whereas Japan has implemented years ago a lasting national programme, RACE, which also covers the generation and accumulation of materials chemistry data.

It is well possible to recover in a concerted action the lost competence of Europe. Simple networking with exchange of people only can no more turn the situation.

For Europe it is required to establish "Knowledge building Structures", with participation of the remaining centres and the active Europe-based Communities which have taken the initiative in their hands.

For many simple alloys and blends a large amount of constitutional information is to be found in data-bases and reference books although frequent revisions and re-assessments are needed. If critically evaluated, such constitutional and thermodynamic data develop predictive power, when appropriate thermodynamic calculation software and model descriptions are applied. Even though such mainly binary and ternary phase diagrams outlined in comprehensive compilations have guided the engineers, their quantitative value is limited because most materials of interest contain many more components and the relevant phase diagrams thus are multi-component.

While considering the science and technology of alloys and blends one has to insist on the fact that assessment, evaluation (possibly also prediction) of multi-component phase diagrams should be one of the first steps, to be followed by (or combined with) the evaluation of kinetic data and the investigation of functional properties in the definition both of alloy and blend applications and their stability, synthesis, processing, etc. It is well known, that to this effect, reliable constitutional data should be available for the sub-system of the multi-component alloy system under consideration: in particular well assessed data concerning the underlying binary sub-systems and some characteristic compositions of the ternary sub-systems are certainly needed. Thermodynamic data are therefore of particular interest. There is a need of reliable thermodynamic data in the evaluation of oxidation, reduction processes, combustion-synthesis methods and in mixing/demixing of polymer-based systems, to name just a few. It should be noted that almost all industrial branches could benefit from reliable data and application skills in materials chemistry.

Experimental thermo-chemistry of alloys has a long fruitful history, but not only in view of the requirements of its applications, but also for several intrinsic reasons as instrumentation, intercalibration, standardization, systematic collection of data consistency of data, etc. It cannot

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be considered to be at all a mature level. The same holds true for polymer blends and macromolecular microphase-separated systems.

The materials interesting in view of new applications are generally based on multi-component systems. Since a complete experimental mapping of such multi-component, i.e. multi-dimensional phase diagram is out of question, computational phase studies known as CALPHAD (Calculation of Phase Diagrams) method are of increasing importance. It offers a very efficient use of the available experimental data and allows accurate estimates of phase equilibrium relationships and thermodynamic properties from a limited set of experimental data.

This means a winning strategy in the investigation of such materials should be based on the coupling of selected high quality experimental measurements of thermodynamic properties with the computational optimization of phase diagrams.

5.1.2. Evaluation of Constitutional Data

A concerted European effort, in which intellectual evaluation of data, targeted experimental and computational phase studies are supported by a modern information technology seems to be the right approach to improve the European position.

With the above figures in mind it is mandatory to have all published information available and to convert the often conflicting data into reliable knowledge. Here, Europe has also a long standing tradition and could rely on MSIT, the Europe based "Materials Science International Team". MSIT is running the world's largest phase diagram evaluation programmes with applied standardization and quality control for 16 years. To make the advanced electronic information system, review and publication structures of this team useful in general seems to be a convincing contribution to improve the European research infrastructure.

5.1.3. Experimental Thermodynamics

An indication of the state of the art in materials thermodynamics may be obtained by considering periodical meetings entitled "Thermodynamics of Alloys" which are organized since 1983 every two years by European laboratories active in this subject. The first one was held in Stuttgart, followed by other centres of excellence in this field, as Vienna, Barcelona, Nancy, Genova, Marseille, Kiel and Stockholm. Generally, mainly European laboratories participated but a few delegates from high-level laboratories from the U.S. and Japan were also present.

In these meetings several hundred communications were presented and discussed. This number is relatively small, as profound experimental work takes time. The increasing power of computational thermochemistry makes the supply of accurate experimental data the limiting factor in searching the large potential of unexamined element combinations. Still numerous experimental difficulties are experienced leaving serious problems in the evaluation and the assessment of data. As a consequence, reliable data, which would be needed for a sound unambiguous definition of the phase equilibria and for a good design of processes, are often lacking.

It can be concluded that in the long history of experimental thermodynamics of alloys, several hundred instruments and methods have been invented, designed and set up in order to determine characteristic temperatures and thermodynamic data. Many papers have been published suggesting and discussing the characteristics of hard (and soft) ware employed in self-made and commercial instruments for data acquisition and elaboration. These instruments and techniques followed and replaced each other apparently, however, without reaching a full technological and methodological final level.

For a certain number of alloy systems (roughly one in every ten binary systems for which a phase diagram has been proposed, a few ternary ones and very few higher component systems) thermodynamic data have been reported. In a very few cases only a complete set of thermodynamic functions (heat capacity, entropy data, formations functions) have been experimentally determined. Although, in a selected number of cases a good reliability may be assigned to the reported data. In most cases this is not true. Heats of formations, for instance, determined for certain inter-metallic compounds by different calorimetric methods in different laboratories very seldom differ from each other by less than 8-10%. Much higher is, on the other hand, the uncertainty and the inconsistency between the values of enthalpy of formation obtained from calorimetry and other methods used for their estimation. As a conclusion it has to be underlined that (due to the great experimental difficulties) there are very few systems for which a complete set of accurate thermodynamic functions is available and can be safely used for subsequent calculations and extrapolations. This is crucial, since all kinds of production of materials, their thermo-mechanical treatment, joining, and their performance in service etc. are controlled

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by these functions. If they are not known, the reliability of processes, components and systems will be substantially reduced. And solid modelling and simulation of production processes, materials structure and property evaluations, which are driving forces for modern technology development, can hardly be performed.

5.1.4 . Computational Phase Studies

In computational phase studies, the Gibbs energy is expressed as a function of temperature, pressure and phase composition for each individual phase in a system including effects of molecular weights and molecular weight distributions in polymer-based systems The mathematical description of phases ranges from the simplest analytical expressions given by regular solution theory, to very complex expressions for phases with several sublattices as well as molecular species, ions and magnetic interactions. The parameters in the expressions are adjusted to quantities that may be derived from the Gibbs energy are fitted to the corresponding experimental data. For example, in a pure element the liquid and the solid phases have the same value of the Gibbs energy at the melting point, the first derivative of the Gibbs energy of a phase with respect to pressure is equal to the volume of the phase etc. The basic idea of the CALPHAD method thus is two fold: it yields a consistency check of experimental data and it offers a scientifically sound method of interpolating and extrapolating the data.

The fundamental thermodynamic treatment of pure elements and substances and the modelling of solution phases have been treated during several international workshops at Ringberg castle in recent years supported by the Max Planck Society. Additionally, the use of computational thermodynamics, especially the CALPHAD approach, for commercial applications was discussed. The general scope was to provide recommendations and guidelines for the development of consistent and compatible high quality and internationally accepted thermodynamic databases. Both, metallic and ceramic materials were treated to test available and new developed multi-component data sets. However, although there is much progress in the thermodynamic modelling, there still remains a lot to be done in order to use this tool for the systematic evaluation of the thermodynamic treatment of materials development process.

Several Windows-based software packages that allow calculation of phase equilibria and phase diagrams as well as other thermodynamic quantities are now commercially available. Calculations considered as cutting edge a few years ago may now be performed on a routine basis by personnel without much expertise in thermodynamics or computations. Nevertheless, such calculations are no better than the databases used and if no data is available for a particular material then no calculations at all can be performed despite the capability of the software.

Therefore, what is outlined in Sect. 5.1.1 is also relevant for computational phase studies. However, a consequent application of computation will be a valuable tool for the planning of defined experimental investigations thus reducing efforts and costs.

Fortunately, good databases are available for some important classes of materials as steels, superalloys and aluminium alloys. These databases cover composition and temperature ranges of industrial interest and their shortcomings are usually well known and subject for further development. For most other classes of materials or compositions far outside the conventional range the situation is much less satisfactory and a large research effort is still needed. This is the case still for many metal alloys but certainly for most of ceramics and polymers and even some types of high-alloy steels. It is unfortunate that it is so difficult to obtain funding for such research. The research efforts need to be directed towards experimental determination of thermochemical properties, e.g. enthalpy of formation of compounds and solutions, activities and phase equilibrium data. The data need to be carefully assessed taking information from all available sources into account and finally represented as Gibbs energy functions that are stored in databases.

Another approach to achieve data is by ab initio computations. Such computations are based on a quantum mechanical analysis of the system and make only use of information that can be found in the periodic table, i.e. no adjustable parameters are introduced. Over the years the computational techniques have been refined and nowadays calculations can often be made with satisfactory accuracy. For example, one may mention calculations of energies not only of pure elements in different crystalline structures but also of compounds and alloys as well as energies of interfaces and surfaces. A drawback is that the calculations are performed at 0 K but nevertheless the results are much valuable. In principle, the calculations give the elastic properties at 0 K and it is then possible to introduce the effect of lattice vibrations and extrapolate the results to higher temperatures. It is expected during the next few years, that these types of calculations are much more common and fruitfully applicable to real systems. In this view a concerted ab initio and CALPHAD-style approach, based on new selected experimental data, has been proposed and should be encouraged.

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5.1.5. Evaluation of Microstructure of Materials

Thermodynamic calculations are often criticized because they yield information only on equilibrium properties, whereas during processing and use of materials the internal reactions, by which equilibrium is approached, are not fast enough to allow full equilibration. This criticism is not always justified. For example, in many cases the situation may be approximated as close to equilibrium with respect to composition and relative amounts of the different phases although a very slow coarsening process may still take place. If certain phases are known to form slowly due to kinetic barriers, a reasonable result may still be obtained by simply excluding these phases from the computation. A metastable equilibrium is thus calculated. An interesting application of large practical interest that requires equilibrium data only, is the Scheil simulation. In this simulation the amount of solid phases is predicted as a function of temperature upon solidification of a melt. At each temperature the composition of the solid layer formed at that temperature is obtained as well as the composition of the residual liquid. The liquid is assumed as being homogeneous at each instant and the composition of each part of the solid remains the same as when that part was formed. For many substitutional alloys this is a reasonable approximation because diffusion in the solid is slow whereas the composition of the liquid should be almost homogeneous due to rapid diffusion and convection. The Scheil simulation makes use of equilibrium calculations only but is able to make valuable predictions on non-equilibrium states.

A more ambitious approach is to combine the thermodynamic calculations with kinetic models, e.g. diffusion calculations, and thereby predict the rate of reactions. This approach is extremely powerful and may be used in future to simulate a wide range of different phenomena, including precipitation, homogenization, diffusional interactions between substrate and coating etc.

It is usually assumed that thermodynamic equilibrium holds locally at the migrating phase between two phases and the rate of transformation is calculated at each instant by solving a set of flux-balance equations. The fluxes are obtained from a numerical solution of the multicomponent diffusion equations.

So far, most of the calculations on realistic multicomponent systems have been made using so-called sharp interface models, i.e. the interface between the two phases is considered as mathematically sharp. This approach has been very successful in predicting growth or shrinkage of precipitates as long as the geometry is simple enough.

However, in this type of calculations the geometry of the particles, i.e. their morphology, is not predicted a priori but rather imposed by the specific model used. The phase-field approach, which has been developed over the last decade, is based on the diffuse interface concept, i.e. the phase interface has a finite width and the properties vary gradually from one phase to the other. These materials properties have not been very realistic; usually binary alloys and ideal solution behaviour have been considered. Nevertheless, the phase-field method is capable of treating multi-component alloys with realistic thermodynamic and kinetic properties and it is straight forward to take anisotropy, elastic stresses etc. into account as long as the computational work can be afforded. In the future it is expected to see simulations where the evolution of microstructure of multicomponent alloys is predicted for various processing and usage conditions.

From the above section it is obvious that high-quality databases are needed also for kinetic properties, e.g. diffusivities, in order to make accurate simulations. In an alloy system with n components $(n\text{-}1)^2$ diffusion coefficients are needed to give a full description of how the concentration profiles evolve in time. A complete description of the diffusion behaviour, i.e. including the Kirkendall effect, requires diffusion coefficients that depend on temperature and composition. The evolution of the concentration profile in a binary diffusion couple may thus be predicted by means of one diffusion coefficient only but already for a ternary alloy 4 diffusion coefficients are needed. The number of diffusion coefficients thus becomes very large in multicomponent alloys and a full experimental mapping is out of question. It is necessary to assess experimental information in a more efficient way that allows the results to be readily extrapolated and applied to new materials. This is possible because the various diffusion coefficients are related to the individual atomic mobilities and the thermodynamic properties. As there are only n mobilities in an alloy with n components it is more efficient to store mobilities rather than diffusivities in a database. The mobilities may be represented by mathematical expressions derived from models of the diffusion process and the parameters in the models may be adjusted until the model is capable of representing the experimental data. This approach, thus, is very similar to the CALPHAD approach for handling the thermodynamic properties and should in fact be regarded as a natural extension of the CALPHAD method. Over the last couple of years several assessments of mobilities along these lines have been presented.

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5.1.6. Future Visions and Developments

A future joint, high quality aimed experimental research effort will be related to a powerful information platform. With a content (or knowledge) driven research and such a information-platform available as administrative tool it should be possible to link different data bases and to co-ordinate competence from different centres, as they are needed in

1. experimental thermodynamics and constitutional research,
2. computational thermodynamics and kinetics,
3. intellectual evaluation of data and diagrams,
4. property measurements and analytics.

These methods normally have to be applied several times in each study. Which method will disclose most of the materials characteristics next, depends totally on the type of material and the state of knowledge achieved.

This research infrastructure could be used to train industrial engineers or Post Docs how to apply materials chemistry most efficiently in targeted materials development, as the "MSIT Training Network on Materials Constitution" successfully did under the former Human Capital and Mobility Programme.

The same research infrastructure could also be used to clarify and generate data for important categories of alloys, relevant to European industry, as the European Action Cost 507 successfully did for the light metal industries.

A joint co-ordinated European effort is highly needed for instance for a systematic programme of:

1. intercalibration of data obtained with the same experimental method in different laboratories,
2. intercalibration of data obtained with different experimental methods, and
3. check on the basis of phase equilibria calculations, of the internal consistency of all the experimental data of binary, ternary alloys of selected multicomponent systems.

Parallel measurements carried out in different laboratories with the same (or different methods) on the same samples should be promoted. Joint decisions about the best instruments and methods to be used and the selection of systems to be evaluated and studied should also be encouraged. A continuous comparison and critical intercalibration of the techniques and of the results is necessary.

It has been underlined that an improvement of the methods and of the instruments, and especially a better standardization of the techniques and the systematic use of, as many as possible, auxiliary analytical techniques would be very useful. Of special interest could be the design and developments of instruments which, with the necessary facilities, could work in different laboratories and routinely at high temperatures.

High temperature, thermal and thermodynamic measurements could be very conveniently inserted in a wider system of high temperature researches, including for instance high temperature microscopy, high temperature diffractometry, etc. Very interesting (not only for equilibria but also for kinetic investigations) could be the combination of high temperature techniques with the use of high intensity (synchrotron) X-ray sources for diffractometry.

5.1.7. Needs and Recommendations

Laboratories dedicated to the above topics do exist in Europe, their level is generally high. The interconnection between the different groups proved to be successful on many occasions, too. Experience in content management and in running large scale materials science teams are at hand as well. The creation and diffusion of information, however, may be largely improved.

What seems to be missing is strict co-operation, all year round, remotely and by personnel exchange; a co-operation which is to be validated by the increment of reliable, applicable knowledge.

What seems to be lacking in Europe is a continuous modernization of instrumentation, and a close co-operation including personnel exchange.

It is therefore highly desirable to create a European institution with the responsibility and authorization to suggest and coordinate research in materials chemistry. The chair or presidentship of such an institute could be assigned in turns to the partner institutions active in this materials network. Students and researchers exchange between all the laboratories involved should be promoted as well as periodic meetings for the exchange of information, samples, planning of future researches, etc.

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In any case it would be vitally important that the material science community in Europe can make use of an electronic steering and communication system

1. that gives access to present, past and future data in materials chemistry,
2. that monitors progress in and outside Europe,
3. that can host and interconnect different databases which remain under the responsibility of the creating laboratories,
4. that reports on ongoing work elsewhere,
5. that serves as an editing tool for joint documentation and publishing.

The system should be platform independent for easy migration to different computer systems and should be permanently maintain data integrity and availability. Most attention has to be given to the management of such a system, as this is the interface between humans and an electronic network.

5.2. Phase Transformations

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5.2.1. Introduction

The specific properties of materials, and thereby the performance of workpieces in practice, are largely determined not only by the intrinsic properties of the materials but to a very large extent by their *microstructure*. A classical example is steel, where only after dedicated heat treatments, bringing about complicated phase transformations, the specific, looked for (mechanical) performance is achieved. Understanding and control of phase transformations in general is a prerequisite to optimize the microstructure with respect to the desired properties not only phase transformations in the bulk are important. Hence it is imperative to have knowledge of the thermodynamics and kinetics of phase transformations in the bulk and at interfaces and surfaces.

5.2.2. State of the Art

Experimental techniques to observe the microstructure are available for the interesting length scale (1 Å to 1μm). Further, a wide range of techniques and facilities are available to study Solid-Gas, Solid-Liquid and Solid-Solid (S/V, S/L, S/S) inter-phase reactions under ultrahigh vacuum or controlled environmental conditions. Sophisticated characterization facilities allow to quantify the structure and properties of S/V, S/L and S/S interfaces at the atomic and electronic levels, e.g. field-emission high-resolution transmission microscopes and various scanning probe microscopes.

A detailed theoretical framework for quantifying the structure, mechanisms, kinetics and thermodynamics of S/V, S/L and S/S reactions, both on microscopic (phenomenological) and atomic levels has been worked out.

A significant amount of atomistic, thermodynamic and kinetic data are available for modelling phase-transformation phenomena to compare between theory and experiment, particularly in the case of metal alloys of components with face-centred cubic lattice e.g., Cu, Ag and Au.

5.2.3. Trends and Expected Needs

(a) Materials

Materials such as ceramics, intermetallics, semiconductors and polymers have growing impact in today's research activities because of their increasing potential for technological applications, relative to metals.

(b) Data

More basic thermodynamic data of the multicomponent materials, such as enthalpies, free energies of formation, heat capacities, interfacial energies and phase diagrams,

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are needed, at least as a function of composition and temperature. Data of thermophysical properties like diffusivity and viscosity are further required to understand and to model inter-phase reactions. The data should be evaluated and easily be accessible. This requires hard work, which is often not appreciated within the scientific community.

(c) Knowledge

• Nucleation

Quantitative prediction of nucleation is the hardest problem in the modelling of interphase reactions. The problem has several aspects. Experimentally, the phenomenon is stochastic and is usually heterogeneous (i.e. catalysed by, often unknown, impurities). The main theoretical difficulty is the calculation of the work necessary to form a critical nucleus. The principal unknown here is the energy of the interface between nucleus and matrix. Determining this energy is particularly difficult in the case of nucleation from a liquid, since the interface is difficult to access experimentally, and modelling of its structure and thermodynamic properties is complex.

• Interface and Surface Energies

Surface and interface energies play an important role, for example recognizing the increasing importance in small scale structures. Unusual (as compared to bulk materials) phenomena can be observed: favourable interface and surface energies can stabilize amorphous phases or, generally, phases that would be unstable as bulk material. Thereby exciting new electric, magnetic and mechanical properties become accessible for practical applications. The thermodynamics for such systems need to be developed, because at the moment only at best semi-empirical approaches (e.g. on basis of the Miedema approach) are available.

• Kinetics

Reactions at surfaces and interfaces and within the bulk are decisive for the resulting properties of materials. One of the great challenges is to find the relation between the thermodynamics (driving force) and the kinetics of the solid-solid, solid-liquid or solid-gas reactions/phase transformations involved. At the moment at best rather bad founded, descriptive, fit functions are used, e.g. the Johnson-Mehl-Avrami function. This should be a main field of future activity.

• Structure of and Reactions at Grain Boundaries, Interfaces and Surfaces

In general, improving our knowledge of the structure, segregation behaviour, mobility and thermodynamics of interfaces, both in equilibrium and in the undercooled or supersaturated states, is essential to progress in the modelling of inter-phase reactions. It is imperative to know more about how the properties vary across inner interfaces of a single phase and interfaces between different types phases.

Some very fundamental questions related to the mechanisms of phase transformations are unsolved, e.g. the mechanism of grain-boundary motion and its relationship to the so-called grain-boundary mobility and its dependence on the grain-size distribution are not even known for pure metals. The role of impurities (segregants) during the processing of materials and the mechanisms by which they affect the resulting material properties are not well understood.

Catalysis of reactions at surfaces is of great technological importance. Catalysts represent a widely utilised class of functional materials where the structure over the whole length scale, from the atomic arrangement to the microstructure, has to be optimized. Each catalysed reaction exhibits many elementary steps from which one step (the reaction-rate determining step) is not in equilibrium. The catalyst works on this elementary step to modify the overall reaction rate. This step is (usually) not known and may change for the same reaction under different external conditions.

• Structure of Liquids and Glasses

Finding a paradigm for the structure of simple liquids that is as simple and compelling as the "periodicity" is for crystals or the "diluteness" for gases remains one of the foremost challenges in science. The concept of "polytetrahedrality", which captures the essential short-range order, comes closest, but even its most advanced formulation only involves a limited number of atoms. Metallic glasses, even though they are alloys, are structurally most closely related to simple liquids. The recently discovered bulk metallic glasses, which can be obtained at low cooling rates and held above their glass transition temperature without rapid crystallization provide unique opportunities for the study of the glassy state. Inorganic glasses are of considerable interest. For example, detailed structural knowledge of the 2 nm thick silicon-oxynitride glass layer found between sintered nitride grains is essential for creating a predictive model for the sintering process.

(d) Materials in small dimensions

Material systems continue to decrease in size. This development is in particular driven by the developments in the microelectronic industry and by the application of surface modifications. The focus on small scale structures, which can be well illustrated by the ever growing importance of thin film structures, highlights a strong need to understand the fundamental relations between the structure and the properties of materials: extreme control on a very local,

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small scale becomes imperative from an engineering point of view, but in particular also from a fundamental scientific point of view, as the properties of small scale materials can deviate strikingly from those of bulk materials. By studying the properties of small scale structures new, fundamental insight into the physics and chemistry of solids is acquired.

Small scale structures, as thin films, are invariably and usually severely stressed. A strongly growing interest in the role of such stresses exists. This is partly caused by practical aspects (as the undesired detachment of a thin layer), but especially also by the associated fundamental aspects:

- The (driving force for) diffusion in small scale structures can be affected strongly by such (nonhydrostatic) stresses, as also holds for the process of electromigration. This is an area of strongly deviating opinions and results. It would be very rewarding if such work would be promoted.

- The thermodynamics and kinetics of phase transformations in a state of stress are hardly understood. Much work is needed in this area, in order to master small scale structures.

(e) Computational materials science; bridging the length scales

In recent years the role of computer simulations to model phase transformations has gained more and more importance. The reason is that is is impossible to arrive on the basis of first principles for the atomic mobility at predictions for the behaviour of an aggregate composed of many crystals. Thus, for example, Monte-Carlo type of approaches can be applied to model solidification (see Fig. 5.1).

Multiscale calculations in time (picoseconds to seconds) and length (atomistic to micrometres) are important in a hierarchical modelling from atomic processes to phenomenological modelling of e.g. phase equilibria and microstructure development. The task is to find the connection between discrete (atomistic) models and continuous models. This is a topic of extreme importance in Materials Science. Recognizing that it is impossible to arrive at an *ab initio* determination of materials behaviour, one realizes that this area of mesoscopical materials science bears great promise, as it appears to be the appropriate and also feasible route to model, for example, the mechanical behaviour of a thin film due to the collective response of all dislocations in the film to some external action. To this end in particular computer simulations and experiments on small scale structures are necessary.

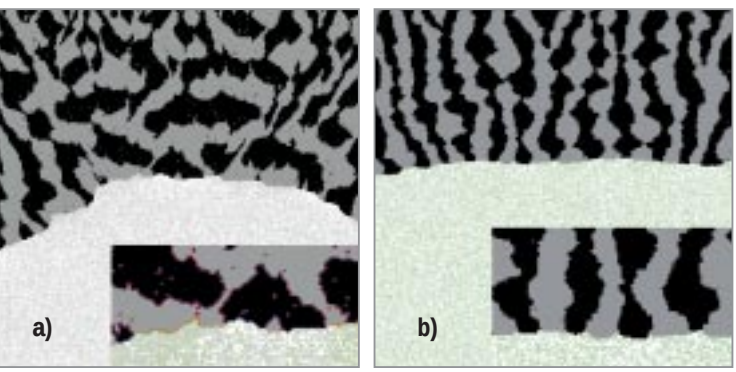

Fig. 5.1. Computer simulation of the effect of surface rearrangement on the morphology of the eutectic solidification structure. No surface rearrangement is allowed in (a), while (b) presents the structure developed with a certain value for the surface diffusion-length parameter. Inset shows magnified view of the solid(top)-liquid(bottom) interface.

5.2.4. Differences in Trends and Needs between Europe and the Rest of the World (U.S. and Japan)

The overall expected trends in basic materials research are similar in Europe, the U.S. and Japan. Research on all types of materials will continue to increase, requiring a comprehensive understanding of inter-phase reactions in these materials. The need for materials scientists to understand and deal with all types of materials will therefore increase as well.

Equipment which is able to sense and respond to processing conditions will be needed to control S/V, S/L and S/S reactions to extremely accurate level in order to reliably produce nano-scale structures. Investment in technical expertise, the development of sophisticated novel equipment and systems is needed to accomplish this goal.

The educational system in Europe is highly competitive with the rest of the world, including U.S. and Japan. There are, however, many more material science departments in the U.S. than in Europe and these perform much of the fundamental materials research, in addition to research in national laboratories.

Europe has a better technical base, i.e., many more highly trained technicians, for supporting basic materials research than countries such as the U.S. and Japan. This is extremely valuable to fundamental research and it should be continued.

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5.2.5. Current Competitiveness of Europe

Europe is competitive with the U.S. both technically and academically. This is true although the amount of fundamental research in some areas such as S/S reactions decreased dramatically for a number of years in Europe. To a certain extend this has also occurred in the past ten years in the U.S., while the opposite has happened in Japan. As a result, Japan is leading the world in a number of areas of materials properties, in terms of both manpower and facilities.

5.2.6. Recommendations

The EU should actively seek to prevent the erosion of fundamental materials research on interphase reactions in the areas described in the above section "Trends, expected needs", in order to maintain international scientific and technological competitiveness. Technology constantly changes, often in unpredictable ways; it can be very detrimental to the natural progression of fundamental knowledge if it is made to follow technology to closely.

There will be a continuous need for investment in state-of-the-art facilities such as sophisticated equipment for fabricating materials, (micro)structure analysis, and computation, etc. Trained personal to maintain and operate the equipment is a prerequisite for successful research in materials science. The state-of-the-art equipment is costly, but it is absolutely essential to remain competitive in science, access to such facilities is a must. It may prove both financially and scientifically beneficial, to establish shared research facilities for major equipment and to provide appropriate travel funds and infrastructure to facilitate their use by scientists in the EU.

Many common phenomena are involved in S/V, S/L and S/S reactions. However, the different scientific communities which study interface reactions often do not communicate and co-operate. It would be useful to establish a strong network of multinational research centres in the areas of materials science that are considered most urgent (e.g. the field of "materials in small dimensions"; see above), where researchers would investigate and exchange information on their progress. Such centres would include both experimental and theoretical groups. These centres would provide more permanent research opportunities for Ph.D. students and post-graduated materials scientists.

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5.3. Interface Science

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5.3.1. Introduction

The goal of Interface Science is to facilitate the manufacture of technological materials with optimized properties on the basis of a comprehensive understanding of the atomic structure of interfaces and their resulting influence on material processes. Of course, establishing such a complete understanding would be a monumental undertaking. Consider the parameters which govern interface structure and behaviour; besides the crystallographic and compositional variables which define a polycrystalline system, the external conditions, temperature, stress, electric/magnetic fields, radiation and chemical environment, prevailing historically and currently need to be taken into account. A polycrystal may respond to such external disturbances by inhomogeneously activating a multiplicity of processes, and consequently the interpretation of experimental observations and theoretical modelling may be correspondingly challenging. In a short article it is not feasible to review the 'state of the art' of interface science in depth, and the reader is referred to the outstanding text by Sutton and Balluffi [1] for a fuller account. In section 2 we outline the crystallographic and thermodynamic foundation which has been established in this field before highlighting the most prominent experimental techniques and some findings from modelling. Subsequently, a representative illustration of the current position in Interface Science is addressed through a case study of interface mobility in

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metallic materials. Section 3 describes recent trends in research activity and future developments that would assist progress. Finally, in section 4, we briefly compare the competitiveness of Europe versus the U.S. and Japan.

5.3.2. Current Position

(a) Crystallographic and thermodynamic foundation

A rigorous crystallographic and thermodynamic foundation is essential for effective communication within the multidisciplinary international community. Following contributions from many researchers, this has been established, and is set out in reference [1] for example. The spacegroup symmetry of any candidate bicrystal (or tricrystal etc.) can be classified in a scheme which takes into account the spacegroups and relative orientation of the adjacent crystals, the orientation of the interface plane, the relative position of the crystals and local atomic displacements. This classification scheme applies to heterophase and homophase boundaries, and colour symmetry has been found to be useful in the latter case. It is conceivable that non-classical symmetry groups, as observed in quasicrystals, could be relevant to interfacial problems, but this possibility has not been developed beyond basic notions so far.

Thermodynamic considerations of interfaces are based on the method introduced by Gibbs, and the reader is referred to reference [1] for a concise review of the subsequent developments in phenomenological and statistical-mechanics approaches. According to Gibbs, interfaces are not thermodynamically autonomous regions, i.e. should not be viewed as independent phases existing in equilibrium with surrounding material. Instead, their influence on polycrystals is treated as a perturbation of the system and is expressed in terms of excess thermodynamic quantities. This formulation emphasises the complex interactions that may occur between material at the interfacial region and in the bulk of the adjacent crystals. For example, impurities may segregate to an interface at lower temperatures, and desegregate at higher ones. In general, the contribution of the excess free-energy due to the presence of interfaces to the total free energy of a polycrystalline aggregate depends on all of the internal degrees of freedom of the system and the environmental conditions mentioned above. Moreover, its significance may change as a microstructure evolves during manufacture or service. For example, the magnitude of interfacial energy may be a key parameter in the nucleation stage of a new phase, but may be dominated by other factors such as strain energy at later stages of growth.

(b) Experimental techniques

A wide range of physical techniques has been employed in Interface Science. Interfaces, being buried structures, are inevitably more problematic to investigate than free surfaces. Nevertheless, much valuable information has been gained by microscopical studies of surfaces. For example, scanning electron microscopy (SEM) has been adapted to study mechanical phenomena such as relative grain motions in polycrystals, electrical features like carrier depletion regions, and chemical concentrations in the vicinity of interfaces. In principle, interfacial excess free energies, relative to some reference, could be found from studies of thermal grooving, but only pilot studies have been reported so far. A major recent development has been the automated use of electron back-scatter diffraction (EBSD) which enables phase identification and grain orientation determination. Instruments are being developed which enable textural information to be gathered simultaneously with *in situ* heating and deformation. Two other techniques that provide valuable chemical information, X-ray photoelectron and Auger spectroscopy, are applied to exposed surfaces following intergranular fracture induced in high vacuum. The performance of the atom-probe field-ion microscope has continued to be refined, and is capable of revealing structural and chemical information at the atomic level by sequential removal and analysis of the surface layers of a needle-like specimen.

Transmission electron microscopy (TEM) is the most effective technique for directly revealing the structure and chemistry of interfaces. The principal imaging modes are diffraction contrast (DC) and high-resolution (HR), and crystallographic information can be obtained using diffraction. Chemical assessment can be carried out by analysis of emitted characteristic X-rays or electron energy loss spectroscopy (EELS). A small number of *in situ* studies of interfacial processes have been published, for example penetration of interfaces in Al by liquid Ga, and phase transformations. Investigations using DC imaging have revealed much about the defect structure of interfaces, giving impetus to the development of defect models of interfaces (see below). In addition, very precise measurements of the relative position of adjacent crystals have been made. HR imaging has elucidated the structure of interfaces in a wide range of materials, and the recent introduction of the z-contrast method enables chemical species to be differentiated. Contrast observed using DC and HR imaging generally needs to be interpreted by reference to computer simulations generated using the dynamical theory of electron diffraction. A serious constraint is that HR imaging requires the incident beam to be parallel to low index directions in both crystals simultaneously, and also to be parallel to the interface plane. Its application is therefore

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limited to interfaces with appropriate crystallography, and cannot be used to investigate less ordered interfaces, an important category about which our knowledge is limited.

(c) Modelling

Topological models of interfaces have been developed on a purely geometrical basis. The underlying notion is that interfaces exhibit regions where the adjacent crystals 'match' separated by regions of 'mismatch'. The regions of mismatch are regarded as defects superimposed on some reference structure corresponding to the matching regions. The defect content in such interfaces can be expressed precisely using the Frank-Bilby (F-B) equation. Initially, this equation was formulated by taking only the translation symmetry of the adjacent crystals into account, and identifying the total Burgers vector, b, intersected by a probe vector lying in the interface. More recent work, based on the Principle of Symmetry Compensation, has generalised the F-B equation by considering the complete space group symmetry of the two crystals [2]. Reference structures can either be a single crystal or some nominated bicrystal structure. The former case is valuable for describing low-angle grain boundaries as arrays of crystal dislocations separated by regions of distorted single crystal. The latter case is helpful for a variety of other interfaces, especially grain boundaries which are vicinal to 'favourable' reference structures, and misfitting epitaxial heterophase interfaces. Arguments using the generalized topological approach have demonstrated that the range of defect types that are admissible in interfaces is broader than previously recognised. In addition, in the case of interfacial dislocations for example, it has been shown that their step height, h, is a second important topological parameter besides b. Step heights can be defined rigorously, and relate to the amount of material transferred from one crystal to the other when a defect moves along an interface. Thus, the magnitude of diffusive associated with interfacial defect motion and interaction can be quantified in terms of b, h and the density of the constituent species in the two crystals.

In general, it is not anticipated that models formulated using geometrical parameters alone can have quantitative capacity for predicting interfacial energies or process kinetics. Consequently, models that couple a physical hypothesis with geometrical arguments have been proposed. A widely used example is the phenomenological theory of martensite crystallography (PTMC) [3]. This theory predicts the displacement, habit plane and shape-deformation for martensitic transformations. The geometrical procedure involves identifying an invariant plane of the transformation, and has been justified on the grounds that such a relationship minimizes the strain energy of a plate shaped precipitate. In general, the habit plane is irrational, and experimental observations are in good agreement with the model for several material systems.

Another model, this time for grain boundaries, is the coincidence-site lattice (CSL) model; the original hypothesis was that atomic occupation of coincident sites at periodic interfaces leads to energetically favourable structures and, furthermore, that such structures exhibit distinctive properties. We now know, from TEM measurements of the relative position of crystals for example, that atomic occupation of coincident sites is exceptional and the proposition has been amended to suggest that periodicity is the key feature. While this notion has not been definitively proved or disproved on fundamental grounds, there is definite supporting experimental evidence in some instances. However, the general applicability of this model is not clear and is hotly debated currently, and the literature is perhaps dominated by advocates rather sceptics. Bollmann introduced the notion of generalized coincidences, or 'O' points. The geometrical part of this theory is equivalent to the F-B treatment of interfacial defect content, but it incorporates the hypothesis that low interfacial energy is correlated with a high density of 'O' points being located in an interface.

Atomic scale modelling of interfacial structure and processes using computer simulation techniques has provided stimulating insights; the reader is referred to Sutton and Balluffi [1] for a review of methods and achievements. Here, we indicate some examples that illustrate the conclusions reached by considering the interactions between atoms. Ochs et al. considered periodic interfaces with identical crystallography in Nb and Mo, and found that the spatial distributions of the conduction electrons in the near interface region were distinctly different in the two cases. Moreover, this caused the relative positions of the adjacent crystals of the fully relaxed interfacial structures to be different in Nb and Mo, as was confirmed experimentally using HR-TEM. Rittner and Seidman showed that segregation of impurities to interfaces in metals is complex and is not simply correlated with geometrical parameters such as periodicity. Misfitting substitutional species occupy sites in the interfacial region in a manner dependent on the details of an interface's displacement field. Cottrell has discussed the strengthening of grain boundaries in Fe by segregation of interstitial C atoms that thereby promote the formation of covalent bonds at the interface. Furthermore, he contrasted this with the embrittling tendency of substitutional O atoms which tend to form ionic bonds. Thomson et al. showed that the consequences of Ga segregation to grain boundaries in Al cannot be explained by hard-sphere arguments. Ga replaces Al at 'tight' interfacial sites, but in a manner which keeps

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the interface structure 'open', thereby enhancing diffusion and mobility. Serra et al. demonstrated that the interaction of crystal dislocations with intefaces in hcp bicrystals under the influence of an external stress is complex. The detailed structure of an interface governs whether incoming dislocations decompose into interfacial defects, become delocalised in the interface, or are transmitted through the interface. Fan et al. studied the variation of grain boundary structure in Al with increasing temperature. They concluded that the interfacial material undergoes structural transitions; for example, at low temperature atoms vibrate harmonically about their equilibrium positions, but at higher temperatures atoms become mobile and more disordered interfacial structures arise. One point, however, that should be recorded is that, overwhelmingly, computer modelling has been carried out on planar 2-D periodic interfaces, and hence our understanding of less orderly interfaces has not been enhanced.

Multiscale modelling [4], in which microstructural evolution or some process such as crack propagation in a polycrystal is simulated, is a valuable research tool. Remarkable correspondence with experimental observations has been obtained in the study of precipitation in superalloys for example. These models are based on phenomenological thermodynamics with order parameters and interfacial energies included in the input data. Crack propagation studies involve the consideration of events at the atomic scale, as well as microscopic modelling of plasticity at the crack tip and also longer range elastic stresses and processes such as diffusion. Deformation of polycrystals with grain sizes ranging from millimetres down to the nanoscale has been studied. These works have indicated that deformation occurs primarily at the interfaces in nanomaterials, and the Hall-Petch relationship between yield stress and grain size breaks down. Such multiscale investigations are very promising, but depend on our capability to identify the key structural features and processes at each length-scale.

(d) Case study: interface mobility

Interface mobility ranges from the speed of sound, as in the case of martensitic transformations, down to values lower by a factor of the order 106 in processes like secondary recrystallization, and can be even slower in diffusional phase transformations. This enormous range reflects the variety of driving forces and interfacial mechanisms that can arise. In the martensite case, the transfer of material across the interface is a shear-dominant athermal process without diffusion and only minimal shuffling. Mechanistic models involving localized interfacial defects are proving helpful in this context, and resemble those in the related process of deformation twinning. This is in contrast to grain boundary motion driven by interfacial curvature which is a thermally activated stochastic process. In a series of outstanding experiments, measurements of interface velocities moving under the influence of a constant driving force have been made by Gottstein and his collaborators [5] as a function of temperature and crystallographic variables. Atomic scale modelling using molecular dynamics has been carried out in parallel, and close correlation was found between experimental and simulated velocities. These studies indicate that low-angle boundaries are distinctly less mobile than high-angle ones. Moreover, in the high-angle regime, the researchers conclude that the activation energies for motion of CSL boundaries are lower than for alternatives, and that the pre-exponential factors are also smaller for CSL boundaries. As a consequence, the mobility of a CSL boundary may be higher or lower than a more general boundary, depending on the temperature. It is apparent from this example that the combination of carefully designed experiments and parallel atomic scale is very effective. In these experiments, a single interfacial process is activated at constant driving force in specimens with known crystallography, and precise measurements of interface velocities are recorded. In the simulations, the motions of individual atoms across the curved interface can be followed, although descriptions of this stochastic process are difficult to summarize except using phenomenological thermodynamic terms. It should also be noted that the role of trace impurities was not established in the experiments or represented in the calculations.

5.3.3. Trends and Needs

Trends in research activity in the field of Interface Science are stimulated by developments in experimental techniques, advances in theoretical methods, and funding policies. With regard to the latter, a balanced support of both basic and applied research is important. Steady progress towards a comprehensive understanding of the influence of interfaces on materials requires an interdisciplinary and interactive effort by researchers addressing issues from the atomic to the macroscopic scales. Collaboration between teams and carefully planned programmes involving experimental and theoretical aspects are likely to be particularly beneficial.

Regarding recent trends in the development of experimental techniques, particular mention should be made of the increasingly widespread use of EBSD. Statistically impressive quantities of crystallographic information can be accumulated with precision, and correlation of this with *in situ* studies of processes such as deformation, recrystal-

lization and stress-corrosion cracking will be valuable. It would also be particularly helpful if such information could be correlated with experimental determinations of interfacial energies, and the role of triple junctions in polycrystal processes. In the field of TEM, instrumental developments that will improve resolution still further are anticipated. EELS promises to advance our understanding of the electronic structure of interfaces and phenomena such as embrittlement, but certain operational problems that currently complicate the interpretation of results need to be addressed. The technique of holographic imaging could provide valuable information about electric fields near interfaces.

The topological model of interfaces is helpful for describing structures and processes, and it is important to recognise the capabilities and limitations this approach. Dislocation descriptions are widely used, but there is sometimes a lack of rigour in published accounts and this has caused some confusion. Similarly, in the reviewer's opinion, there is a lack of critical appraisal regarding the general applicability of the CSL and 'O' lattice models.

As outlined previously, atomic-scale and multiscale computer modelling is providing valuable insights into interfaces, and they are likely to be particularly helpful in future if carried out in support of experimental studies. Although some aspects of these calculations are sophisticated, much development is needed to progress a broader understanding. For example, in the case of homophase interfaces, there is a need to study more disordered interfaces that will require the use of periodic boundary conditions in the calculations to be circumvented. To date, relatively little work has been done on interphase boundaries where additional theoretical challenges arise. The success of multiscale simulations depends critically on the information input, and the identification of key structural features and processes. In this latter respect, physical processes need to be expressed in a framework that links different length scales. As an example, we cite the calculation of the diffusive flux of material associated with motion of an interfacial dislocation, as was mentioned previously, in a simulation of a phase transformation. Diffusive fluxes might extend over mesoscopic dimensions, but are quantified in part in terms of the microscopic parameters b and h associated with a transformation dislocation. In the context of martensitic transformations, rather than diffusional ones, such fluxes must be nil. In stiff materials like metals, it has been demonstrated that this condition can only arise when the heterophase interface is an invariant plane, thereby giving a mechanistic insight into the phenomenological model of martensite formation. One can foresee multiscale simulations in the future that incorporate these notions and hence enable the influence on the transformation kinetics of further factors, such as the density of dislocations in the matrix phase, to be assessed.

5.3.4. International Standing

To a certain extent, the Interface Science community is international; research output is published in the open literature and conferences are often organized on an international basis. The European contribution to this international effort is comparable with those of Japan and the U.S., although some characteristic differences are evident. All three groups have teams of very high quality researchers with active specialists in all the key experimental and theoretical activities. The individual teams are well founded and relatively stable, and are based in a mixture of government, educational and commercial institutions. Collaboration between teams is very important, and European networking is good in this respect. Communication between teams if also very important, and the annual cycle of major international meetings held in the U.S. is the most active. There is a history of financial support for both basic and applied research in all three groups, although there has been a trend towards more applied work in recent years in Europe and a decrease in the research output of commercial organizations.

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5.4. Nanomaterials

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The promise of nanotechnology: "So powerful that it will allow desktop manufacturing… So portable that everyone can reap its benefits… So radical that it will change our economic and political systems… So imminent that most of us will see its impact in our lifetimes."
Kai Wu, Cornell University.

5.4.1. Introduction

The march towards miniaturization carries on at a relentless pace. The promise that one can obtain more for less, produce smaller, lighter, cheaper and faster devices with greater functionality while using less raw materials and consuming less energy is beginning to be realized. This promise derives from the world of nanoscale science. It's a world which also promises better electronics, computers, communications, improved medical diagnostics and treatments, better environmental sensors and less pollution.

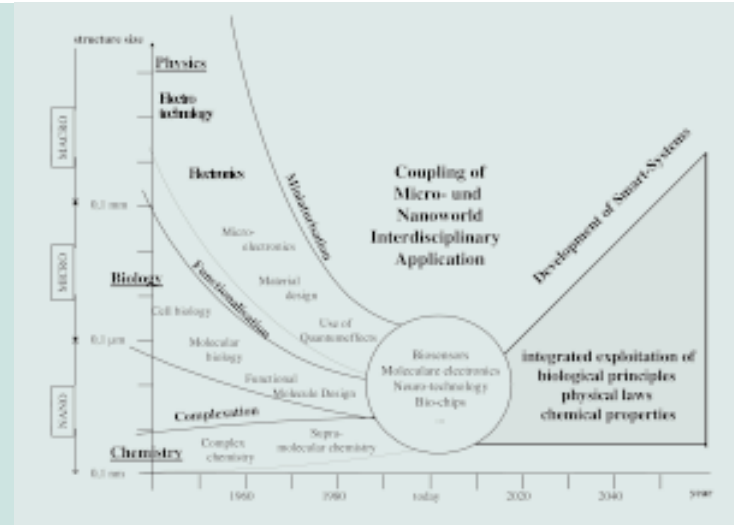

Fig. 5.2. Technology Forecasting – courtesy of G Bachman, BMBF, Germany.

The nano world is defined as a technology in which "dimensions and tolerances in the range 100nm to 0.1 nm play a critical role".

The field of nanotechnology and nanoscience is, by definition, extremely broad and covers everything from electronics, sensors, healthcare and personal care products etc. through to micro electronic mechanical machines (MEMS). This nano world is not just a promise of greater things to come – though it will undoubtedly be a major factor in the wealth creation and quality of life of future of future EU citizens, but is here with us now. The opportunities for industry across the EU are immense as well as being extremely varied and exciting (Fig. 5.2). Some have been identified and illustrated in the document published by the VDI in 1998 – "Innovationsschub aus dem Nanokosmos" – "Innovations in the Nanoworld" and in the UK Foresight document – "Opportunities for industry in the Application of Nanotechnology", prepared by the Institute of Nanotechnology (http://www.nano.org.uk) and published by the Office of Science and Technology in April 2000. In addition, a follow-up document "Nanotechnology: The huge opportunity that comes from thinking small" will be jointly published by the Institute, the DTI and Eureka in June 2001. The objective of the latter publication is to demonstrate to industry that nanoscience is already changing the face of materials manufacturing.

5.4.2. Future Visions

We are experiencing the second wave of nanotechnology and nanoscience, where the area has moved on from the fanciful visions of Drexler to the more pragmatic solutions for today's industry(see references). However, the potential of the topic is not diminished, its potential is enormous and is now built on the foundations of a strong materials science base. A large number of the future directions for nanomaterials is outlined in the next section, however it is worth identifying areas that are more futuristic and will certainly warrant future seed-corn funding.

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The science of the nanoscale world is one that is truly interdisciplinary requiring a mix of skills from the physical, medical, biological and sociological sciences. The materials and devices that will appear will come from the development of smart tools with "turn-key" operation and an intuitive interface. These problems will best be solved by consortia including experts in the human-machine interface. It is important to stress that the EU will serve a strategic role by taking the long (>5 year) term view on fundamental research. The shorter term perspective will better and more properly be taken by the growing business community in this area.

Taking this view the area of nano-materials will offer enormous opportunities to the electronics, medical and biological industries. Massively parallel fabrication, perhaps utilizing directed self-assembly or molecular templates [cf . organic growth] could enable the pharma industry to manufacture numerous small amounts of a therapeutic candidate in parallel. This would eliminate the time consuming process of scale-up in the development cycle. To achieve this requires cross sectoral working involving chemists, biochemists, etc whilst topics such as seeding at surfaces and structures using novel lithographic techniques will need to be researched. In addition an architecture requiring a fundamental understanding of 3D assembly of complex molecular structures possibly templated by physical structures is essential. Increasingly important will be the study of 'biological' nanoparticles – that is large naturally derived biological molecules (proteins, peptides, etc.) as nanoparticles and clusters of nanoparticles and how this affects their subsequent properties and interactions with biological materials.

The whole interface between biological systems and functional semiconductors remains a relatively unexplored area that will afford great benefits. The ability of electronic/optical devices to sense minute samples of biological/medical materials *in situ* and to relay this information to a central location opens up possibilities for the remote monitoring of patients. This would remove costs from the health systems of countries whilst at the same time ensuring the patient can exist in the less stressful environment of their own home. The extrapolation to single living cell diagnostics will be important for future preventative medicine.

The extension of Moore's law is expected to continue for the next 10 years with devices in their present form. However, looking to the future then single molecule and single electron transistors will appear. Again there will be a need for the design of complex novel architectures to accommodate these new devices. The materials will be novel as will gate designs and the interconnects.

The need for bigger and faster computers is a given in the future world. That they will not look or perform in the same way as today's machines is taken for granted. This new world will be the world of the quantum computer. Its designs are still being formulated, however, what is known is that it will depend on new materials and compositions to work. If the binary component, Qubit, depends on atomic spin then materials in which this spin can be "frozen" together with materials to read-out the subsequent bits are essential.

A major failing of nanoscience is the lack of understanding of the physics of interaction of objects (surfaces, particles, individual molecules) at the nanoscale. Questions need to be answered regarding how nanoparticles can be stabilized, and in what media, how nanoparticles interact and influence each other, what proportions in a hybrid system make a critical difference. How can these characteristics be predicted?

The need for more and better modelling is becoming imperative. The more of the basic science that can be achieved via machine "experiments", the faster the throughput of new molecular combinations for the production of new materials and nano-structures.

The area of Extreme Nanotechnology requires vast amounts imagination and intuition if nanoscience research is to come to fruition. Its potential is vast and it is proper that the underpinning nanoscience be properly supported. However this should be part of a balanced approach to funding whereby the top down nanoscience and nanotechnology is not overshadowed since the benefits from this area will be considerable in the medium time frame.

5.4.3. Research Areas

Nanofabrication – encompasses the making of things with dimensions less than 100nm and involves lithographic techniques beyond what is possible by optical means. This is building from the top down.

There are several materials issues to consider for lithography moving into the (sub-100nm line-width). In the range around 100nm, stepper technology can be used with phase-shift masks, although the masks are complex and expensive to design and make. In the sub-100nm range there is an assumption that, for the foreseeable future, the basic mechanism for image generation will be either e-beam or X-ray lithography. E-beam is inherently high resolution and (relative to X-ray) lower in capital cost and

materials, but slow as it is a serial technique. X-ray lithography is very expensive in capital outlay (synchrotron sources) and mask materials (X-ray masks require heavy metal absorbers on a thin silicon or nitride membrane). New soft lithographic pattern transfer techniques are being researched. These include "contact printing" using e.g. elastomer stamps. SPM techniques can be used for direct writing of patterns, but are currently very slow. The development of an SPM "toothbrush" with millions of tips would greatly improve the speed of such a technique by enabling parallel-writing.

There are two classes of resists, chemically amplified and non chemically amplified, that can be used for nanolithography below 50nm. For the chemically amplified resists, the materials issue is how to control the acid diffusion in the resist which determines the extent of polymer chain scission or cross-linking. Using chemically amplified resists is recommended because they have very high sensitivity which can considerably reduce the exposure time. Their resolution is limited by acid diffusion and the best result achieved has been 30nm lines. The non chemically amplified resists are inherently low sensitivity but of high resolution capability, and 5-7nm resolution has been achieved with PMMA. At such resolutions, intermolecular forces become the determining factor. The resist molecular size is around 2nm but so far no one has been able to get to the resolution where molecule size becomes the limiting factor. That is because the lithography tools, such as e-beam, have scattering effects which create a latent image in resists larger than the probe size. Clearly, research is needed into higher sensitivity resist materials that can have reduced scattering and do not need chemical amplification.

• Mask materials for nanolithography

New materials are required that can be used to create robust, lower cost X-ray lithography masks.

• Contact printing

If a "master" pattern can be created by using e.g. e-beam techniques, then there may be techniques by which this pattern can be transferred to an other substrate. This has been demonstrated using elastomers, but higher resolution materials for this technique would be interesting. Alternatively, work on (non-elastomer or hybrid) could provide a technique for rapid and low cost multiple transfer of e-beam created images to device surfaces.

• Self-organizing materials

The use of self-organizing (e.g. biological or biological-like) materials could offer a novel method for pattern generation. At the moment such materials do not exhibit the long-term stability or spatial regularity and accuracy necessary for use in industrial processes (e.g. for chip manufacture where layer-to-layer registration is essential). It may be possible to externally-impose order over long spatial distances using more conventional lithographic methods and rely on local order using a self-organising system. Combination of top-down and bottom-up areas of nanotechnology and the materials issues associated with this may have interesting implications.

Many techniques exist for building up materials (both organic and inorganic) at the molecular level. Most of these provide nanostructures in 1 or 2 dimensions. There will be a need to be able to pattern on the nanoscale in 3-D. Technologies need to be developed over a wide range of materials.

Nanometrology – the precise measurement of structures fabricated with dimensions less than 100 nm. It also includes the development of such measurement techniques.

This not essentially a materials issue, however the ability to handle materials what ever their form and state is important, both for nanoscience research and for nanotechnology. For nanoprobe analysis, e.g. using STM/AFM etc then these techniques require the manufacture of tips that are chemically inert, physically stable and can be fashioned reproducibly into atomically sharp points.

The metrology challenges of pushing towards shorter wavelengths on 'conventional' steppers probably remain in the domain serviced by laser interferometers (although the picosecond ultrasound laser sonar technologies may offer an alternative measurement method for opaque nanoscale multilayers). There is some argument for using the lattice of a wafer as the displacement reference (together with a coarser scale etched onto its surface). However, the difficulty of getting strong signals and contrast fringes by using X-ray interferometry for the read-out seems too high. STM, or similar readout, of the reference lattice might just be possible. The technological limits also need to be established. Good mechanical and servo design are the critical issues for next generation steppers. Metrology of nano-artefacts – proving that the nanolithography does what it should – is a bigger technical issue for which there are no obviously dominant technologies. SPMs need better (and traceable) internal metrology. This includes force as well as the main displacement axes. There are still major problems with tip characterization – geometry, chemistry, etc. – for use under industrial conditions. SPMs only deliver atomic resolution on very smooth surfaces. How can the quality of a groove that is supposed to be 10 nm wide and 10 nm deep be assessed? It could be that only electron microscopes can do this, however it is expen-

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sive to get good quantitative information. There is worthwhile research in looking for materials that can give an indirect measure – for example, their response to the structures of interest is to grow (upwards) in characteristic ways that can then be measured with, say, an SPM.

Functional nanotechnology – describes applications in which nanostructures are used to produce improved optical, electronic and magnetic properties.

Moore's law will continue to dominate the electronics industry for the next ten years. The lithographically defined dimensions of semiconductor devices are already close to the 100nm range with minimum thicknesses down to the 10nm range. However, there will be an increasing demand for materials combinations of semiconductor, insulator and metal layers where the dimensions of the layers could be at the atomic layer limit – well into the nanoscale. These materials will exhibit novel functional properties not found in nature and will be dependent on quantum effects arising from the thickness dimensions.

The move to 1D and 0D structures will need to be researched. 1D structures are quantum wires whilst 0D structures are quantum dots. Quantum dots are in themselves nanoparticles with general properties described in the sections below, however, in their semiconductor form they can be produced to give novel optical properties which could find uses across the whole of the IT and telecommunications industry. Manufactured in other materials then novel phosphors may be produced. They could have major applications in crime prevention.

A barrier to the introduction of nanoelectronics, is that there is no established mass production techniques for creating devices. Research needs to be done to establish how a nano three terminal device will be fabricated on a large scale over large areas, in what will be novel materials. The architecture for such processes needs to be established.

What has been described for novel functional materials also needs to be applied to new insulators and metallic structures without which no device can function. New materials need to be researched which will facilitate heat and electrical insulation as well as heat and electrical conduction on such small scales.

One can envisage research at the nanoscale enabling – new high speed MQW devices needed for very high data rates, ultrafast optical switches for all-optical networks, amplifiers that can operate at wavelengths inaccessible to existing erbium doped fibre amplifiers and microscopic optical benches for precise positioning of new optical devices.

Ferroelectric materials offer a wide range of functional properties (dielectric switchability, piezoelectricity, pyroelectricity, high permittivities, strong electro-optic effects etc) in a wide range of forms (polymers, oxides, organic and biological). It has been demonstrated that the effects persist at the nanoscale. It has been shown that ferroelectric thin films can be fabricated which show ferroelectric properties in layers as thin as 2 molecular layers, and domains can be switched and read with a demonstrated resolution of 40nm. Smaller resolutions are probably possible. There are therefore exciting possibilities presented by the use nanomaterials in a wide range of functions, including memories, high frequency filtering, optical and photonic devices etc. Research is required into both the fundamental properties of these materials at the nanoscale and their manipulation and exploitation in this range.

Ferromagnetic materials are of interest for high density archival storage systems. There is some research on systems and their fabrication and this could be a fruitful area for expansion beyond the nanoscience stage.

Organic thin films are as yet largely unexplored by comparison to semiconductor layers. However, constructed in a similar manner they could be fabricated to respond to specific and different organic and inorganic materials. These could find applications in a multitude of sensors and new types of optoelectronic displays.

Chemistry is the basis to understanding and providing unique material properties. An example is the manipulation of conductive and semiconductive compounds, e.g. organic polymers, to increase the carrier mobility (> 1 cm^2 V-1 s-1). This may be achieved by control of the packing, of say the polymer chains, at the nm scale. Molecular wires/rectifiers are a longer term goal, but there are more immediate applications to organic LED technology and generally to 'organic electronics' (smart cards and radio frequency Identity Tags – applications where processing speed are not vital). There may also be implications for the microelectronics industry (spin devices, resonant tunnelling structures, single electron transistors etc.). There are also many non-electronic applications, e.g. fashion industry ('smart' clothes), decorative finishes that respond to environmental changes. Or, one could combine this area with electronics, e.g. wall displays, photovoltaic wall coverings. Novel piezoelectric materials need to be created so as to be "smart", i.e. materials that can both sense and respond to the surrounding environment.

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The development of new fields of science and technology, such as quantum computing, will requires the development of entirely novel materials systems. The importance of this field cannot be emphasized enough.

Nanomechanical devices and machines – an extension of the present day micromachines and microactuators into the nano world.

At present the whole world of MEMS – micro electromechanical systems – uses conventional materials be it silicon, glass or metals. As the dimensions contract progressively moving into the nano world, then different material properties, are needed, especially in terms of their relation to surface properties, whether for lower friction or reduced surface tension. The incorporation of basic self assembly techniques is already occurring, and research needs to focus on building from the bottom up to produce the next generation of nano devices. The possibility of many microreactors or micromachines in a massively parallel operation describing the nano factory of the future becomes an engaging possibility. Nanosensors for force, acceleration, pressure and other measurements will be both demanded and enabled by such developments. Chemical and biochemical nanosensors will also be required and might be made using carbon nanotubes (see later) containing enzymes or electroactive molecules. Molecular motors, such as those used in muscles or bacterial flagellae, may be of use in pumping or controlling fluid flows on this scale.This requires further nanoscience research, however, as does the reluctance of fluid flows to mix at the nanoscale.

If very fast NEMS systems can be made, they could find use as fast actuators where very small forces are required. Tribological issues must be addressed and the use of dry lubricants is of interest because of the surface tension problems which limit wet lubrication. Surface modification by ion implantation has been used in macroscopic applications and it should be considered as part of the armoury of tools for the nanoengineer/scientist.

Molecular nanotechnology – the technology of molecular sensing and molecular recognition. It reflects the interface between the biological/medical and inorganic systems.

In order to create new and more effective biomaterials, work at the nanoscale needs to accelerated. This will lead to the customization of material and surface finish required for a particular application. Characterization of materials at the nanoscale is vital, for example, in prosthetic replacements for bone and teeth where special load bearing strength and biocompatibility characteristics are required.

It is the properties *at the interface of the surfaces*, which can dictate the properties of the material as a whole. Interactions between polymers and organics can be fine tuned, and their performance consequently changed, giving rise to new phenomena as a result. For example, a nylon nanocomposite with only 2% organics exhibits:

- Increased elasticity and strength
- Increased heat resistance
- Increased toughness

Considerable research is required to understand how the chemical composition of materials affects the interface properties, critical to the design of new materials.

It has been also been known for a while that the morphology and topography of a surface dramatically affect the behaviour of living cells on that surface. Further basic research on nano and textured surfaces to understand what makes them cell friendly and encourages cell growth. Directing the growth of nerve cells on micromachined structures is the first step in bio-computing.

The use of DNA, which can conduct electrical signals as well as act as a structural material requires further research, as the basis of many applications including the possibility of making biological robots.

Nano particles are being used for drug delivery. Surface modification of the particle will allow for more effective delivery or target existing drugs. This is a vast materials area for the pharmaceutical sector. Nanoparticles are also being developed as delivery mechanisms in gene therapy – a means of rectifying genetic disorders. Good DNA is inserted into specific sites in target cells to replace faulty genes. Effective particle and materials design is the key here.

Microfluidics are an essential part of the drug discovery and evaluation procedure. Pico and Femto litres of material can be examined in this way. The drive is to reduce dimensions even further and to be able to examine the effects of new drugs on single living cells, or on organelles or viruses, within them. Allied with combinatorial chemistry the whole area of the lab-on- a-chip becomes a viable alternative. Materials properties are essential in that flow and surface tension become critical if this area of sensors is to become commercially viable. The extension of this technology to incorporate micro/nano fluidics with active devices such as semiconductor devices is as yet almost

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unrealized. This opens up possibilities for *in situ* monitoring of patients by remote means. Thus removing costs from the health system whilst ensuring the patient can exist in the less stressful environment of their own home. All of this could be very valuable, but most of it will require substantial nanoscience research before it can be realized.

Particles, clusters and catalysis – on the nanoscale promise new and improved properties capable of producing a multibillion pound industry for the 21st Century that promise even greater innovations than did their predecessor Colloid Science during the 19th and 20th Centuries.

The ability to control the morphology and size of nanoparticles is of fundamental importance, as well as establishing means to stabilize them. Research into modifying the surface chemistry of nano particles fabricated from metals, semiconductors or ceramics to produce multifunctional groupings is needed, as the basis of many new properties and applications (Fig. 5.3).

Further research is needed into nanoparticulate catalysts and the phenomena that affect their reactivity. An understanding of the nature of these active sites has proven difficult but essential. However, an understanding of the effect of the material properties and surface morphology on the efficiency of the process is even more recondite.

The ability to design and mass produce nanoparticles of a given shape, size, size distribution and composition has implications for many aspects of materials science with applications in drugs, cosmeceuticals, coatings, paints, pigments, composites, and lubricants. Depending on the surface modification of nanoparticles, improved, optical, structural, thermodynamic, viscosity, mechanical, absorption, reactivity and magnetic properties can also be controlled.

Nanostructured materials – where the grain and composite size is less than 100nm, offer the potential for stronger, more wear and corrosion resistant materials.

The grain size of materials affects their characteristics. This is related to the large area of grain boundary per unit weight of material. More research into these effects will underpin much of the future applications of materials science.

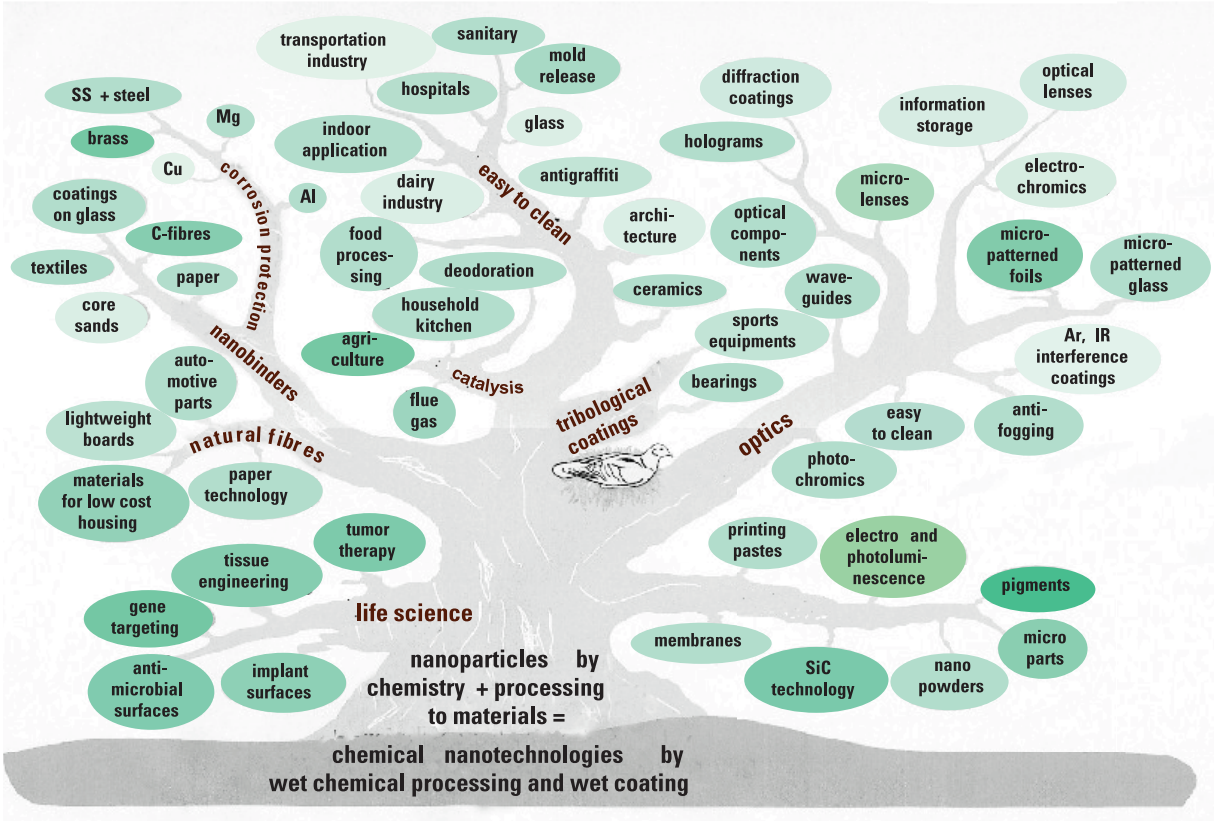

Fig. 5.3. Applications for nanoparticulate research – courtesy the Institute of Nanomaterials, Saarbrücken.

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Presently one effect of nanoparticles is seen in the use of modified clays in plastic composites to give improved strength, heat stability and barrier properties. New composites need to be researched with novel properties dependent on the incorporation of nano-sized materials, and the effects of shape, distribution, volume etc; and the composition of substrate and additive. Composites will have wide range of applications ranging from structural, environmental, healthcare to catalysis.

Further work also needs to be done on nanocrystalline materials to gain an insight into strength and durability characteristics over a wide range of compositions with improved properties of hardness, wear and erosion resistance for tips for nanomachines and devices. Some investigation needs to be undertaken into characterising superplasticity regimes.

The novel use of nanocrystals currently seen in photovoltaic cells demands more research into the type of semiconductor used, which needs to have surface for light absorption and charge separation, and may have major implications for other applications. This offers great promise to enable large scale storage of solar energy as combustible gases.

Other developments in this area include composite material for flat panel displays which could be screen printed over large areas.

"Extreme" nanotechnology – represents atomic and molecular manipulation and assembly. That is building from the bottom up. This field is the most speculative but promises large long term gains.

This area is as yet a white board for novel materials. The challenge is in economic scale up, at as close to ATP as possible. This may be achieved through self assembly, the use of biological techniques, or mass production from arrays of nano tools.

Further research into carbon C_{40}, C_{60} and C_{70} molecules, known as "bucky balls" will lead to a more comprehensive understanding of their properties. The ability to incorporate other molecules into molecular carbon cages could lead to whole new families of novel compounds. Carbon nanotubes are also relatively little understood though their potential uses are considered to be numerous. These include mechanical devices such as probes for STM/AFM etc, to providing novel electronic optical and other functional properties for incorporation into a variety of devices. Carbon nanotubes offer promise as electron field emitters in panel displays, single – molecule transistors, gas and electrochemical storage, catalysts, sensors, protein supports, and molecular filtration membranes.

Further research into self assembly using techniques such as supra-molecular chemistry and how molecules can be arranged into more complex structures has many implications. Designer structures can be formed that arrange themselves into functional entities held together by an advanced "molecular glue".

Biomimetics – copying nature's techniques as a basis for creating materials with novel properties, or using/modifying existing materials produced by living creatures, or using organisms as the basis of novel material production.

Nature has created many materials from which science can learn. Research needs to delve further and emulate nature's processes. Already a novel method of capturing energy by creating a solar cell which is based on how a leaf cell photosynthesizes has been developed. Other lessons can be drawn from the properties of cell walls which can lead to the creation of new thin films with many properties; the strength of shells derived from their crystalline structure and the intercalation of organic films, which can lead to the manufacture of stronger and lighter materials.

Research into the lessons of the biological world will lead to self assembly techniques, biocompatible high strength, lightweight materials, medical glues and sutures that are not rejected by the body, the development of porous structures that can be filled as required, high strength lightweight structures for macro load bearing applications; biological based mass production of designer molecules, novel filters for toxic gases and liquids, scaffolds and so on. Emulating the design of unicellular animals such as foraminifera, diatoms, radiolaria and coccoliths will have implications for the design of nanomachines.

Computer modelling – simulation at the atomic level is needed to understand the new physics of the nanoworld. Through this, performance and chemical/physical characteristics of novel materials may be predicted.

With the increasing possibilities of nanotechnology then the need for more and better modelling becomes imperative. The more that can be done via machine "experiments" enables a faster and more cost-effective throughput of examination of new molecular combinations and nanostructures. This will underpin much of the nanoscience research conducted, be it top down or bottom up.

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At this time the ensemble of modelling techniques form a set of modelling bridges between technology islands. For example electronic (dealing with electrons, eg density functional methods) and molecular (molecular dynamics, Monte Carlo) modelling can make predictions concerning nanoparticles (eg defect electronic properties, wetting properties), or macromolecules. The next level of complexity is where we may have clusters of nano-objects and/or the presence of mesoscale interfaces and where timescales approach microseconds, these methods may be supplemented by mesoscale modelling (eg dissipative particle dynamics, continuous time random walk) methods. This will be important for nano-bio materials (where the key may be molecular but the door on a larger scale), for nanofabrication where we want to manipulate small objects with larger ones, or nano-pattern bulk surfaces; indeed for all of the frontier areas between bulk materials and nanomaterials.

Modelling and simulation in the nanomaterials area is interdisciplinary in that it involves chemists, physicists, biologists, applied mathematics, engineers interested in particular phenomena and applications. The present state of the art is one where existing algorithms are being applied to new nanomaterials, new algorithms are being developed (eg for electronic properties, mesostructures, non equilibrium systems) and new combinations of algorithms explored to bridge the gap between nanoscale properties and the consequences for devices ie for nanotechnology. Research support for all three approaches is required if the full potential for modelling and simulation in nanotechnology is to be realized. As always with numerical computer based methods, one limitation is the speed and memory limitations of existing hardware. One challenge for the future is to utilize the power of grid technologies through software platforms such as Cactus [1] to reduce compute power barriers.

European levels of funding for nanotechnology are lower than in the U.S. Modelling and simulation provides an opportunity to be smarter, quicker. Whilst experimental programmes are vital, high levels of funding for modelling will help to ensure that more value is obtained from experimental programmes than would otherwise be the case. We have an excellent base of modelling expertise in Europe from which to grow this area.

In conclusion, modelling and simulation can play a key role in understanding and applying nanomaterials. By supporting interdisciplinary modelling teams Europe has an opportunity to compete more effectively with the world centres in nanomaterials. One strong recommendation is that European support for nanomaterials research should normally require a significant modelling effort to be an integrated part of the work.

5.4.4 . Place of Europe in the World

In the U.S., as a measure of the interest and commitment by the U.S. government, the fiscal budget for nanoscale science has been more than doubled in recent years:

- For fiscal year 2001 the U.S. government allocated $422M
- For fiscal year 2002 the U.S. government will allocate $485M

Individual States are also investing to ensure that they can share in the prosperity and employment that this will bring, e.g. California has invested $100M to prime the creation of a $300M California Nanosystems Institute.

Similarly, in Japan the importance of nanoscience to their economy is exemplified by the spending of $410M in the last fiscal year and the setting up of 30 university centres with expertise in nanoscale science and technology.

There is clearly a well defined acceptance in the industrialized countries that research at the nanoscale is vitally important for the future prosperity and quality of life of their peoples. The various European countries are investing in nanoscale scientific research, to a greater or lesser degree, but there is little or no evidence of a co-ordinated approach across the whole of the EU. This situation urgently needs to be addressed otherwise Europe will lose the race in this technologically vital area. The opportunities in the materials arena in particular are vast. For example, the market in advanced ceramics alone is expected to reach $11 billion by 2003. Other materials applications include new coatings for data storage, better and cheaper dyes and pigments, lighter and stronger materials for cars, planes and spacecraft and durable anti-corrosive, heat-resistant, water- and even bacteria-repellent coatings (Fig. 5.4).

It is accepted that nanostructured materials have substantially different mechanical, electronic and magnetic properties as compared to conventional materials.

Fundamental research in understanding the basic science is now essential to lay the foundations for exploiting the multitude of opportunities that will be presenting themselves in the near future. We need to know,

- how to modify surface properties of materials,
- how to control the interface composition/structure of multicomponent materials to yield different properties,
- how new multifunctional nanomaterials can be designed for different devices.

The answers lie in pushing our knowledge beyond present limits.

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	1 Medicine/Pharmacy/ Biology	2 Precision Mechanics/ Optics/Analysis	3 Chemistry/Materials
A Fabrication and Application of ultrathin Layers	• Biocompatible Surfaces • Diffusion Layers • Photosynthis Films	• X-Ray Optics • Quantum-Wel-Lasers • Functional Layers (Filtering, Reflection, Minimization, ...)	• Polymeric Films • Gradient Layers • After-Treatment of Layers
	• Sensor Surfaces (Bio-, Chemosensors) • Adhesive Technologies (on variable Surfaces) • Effective Catalytic Surfaces •Corrosion Inhibition Layers		
B Generation and Use of lateral Structures < 100 nm	• Si/Organic Coupling • Medical Nanomachines • Ultrafiltration • Biomoleculare Information Processing • nm-Electrodes/Cappillaries	• Fresnel Optics • Diffraction Gratings • Mechanical Sensors • Lithography Machines	• Particle Filters • Copy Protection • Structuring via Deposition
	• Tip Arrangements (for Photo Detectors, Field Emitter Displays, Electro Filters, High Voltage Switches, Solar Cells,...		
C Production and Application of Nanomaterials and molecular Architectures	• Research on effective Substances • Positioning of Phrmaceuticals • Key-Lock-Material Systems • Nano emulsions	• Frictionless Bearings, Lubricants, Vaccum Rotary Transmission	• Nano Particle Production (Colloids, Pignents, Dispersions, Nano Powder, Nanocrystals, Emulsions, Clusterm Fullerenes,...) • Compound-/Gradient Materials • Supramoleculars Units • Corrosion Inhibitors • Zeolithe Reactors • Weak Magnets / Ferrofluids / Magnetic Particles • Molecular Chemionics • Ceramic Process Technology • Hybrid-, Effect-Pigments
	• Systems of compacted Nanomaterials (Membranes, reinforced Plastic Material, Light Absorber, Aerogels, Light Emi		
D Ultraprecise Finishing of Surfaces		• Correction of Polishing Faults • Optics with nm-Accuracy (Stepper Optics, Aspherical, Substrates for X-Ray Optics, Infrared-Optics, diffractive Optics, Laser Mirrors) • Machines for Precision Engineering	
	• Tools and Methods for the Fabrication and finishing with nm-Tolerances and nm-Form Accuracy (Turning-, Grinding- and Polishing Machines)		
E Measurement and chemical Analysis of Nanostructures	• Research on Adhesion Phenomena • DNA-Analysis • Cosmetic Research • Development of Pharmaceuticals • Analysis of Bones, Skin, Hairs, Teeth • Sreening of effective Substances • Local Action of effective Substances • Cheap Bioanalytics • Analysis of biological Cuts • Analysis of Toxicity	• Components (Profilometer/ Iterfero-meter, Microscopes, Spectrometers, Scanning Probe Tools, Postitioning Components) • Nanolabs (Analysis+Structuring) • Development of functional Tips • Analysis of technical Surfaces • Characterization of Polishing Processes • Form & Finishing-Measurement • Absolutely Calibrating Systems	• Corrosion Research • Single Molecule Analysis • Catalyst Research • Particle and Cluster Analysis • Computer Simulation
	• Broadly applicable Process and Quality Control (for Layers, Particles, Structures, Functions) • Analysis as Presupposition for the Product Development • Analysis as Aid for teh Development of a new Thinking for Applications in the nm-Range		

Fig. 5.4. Industrial Relevance of Nanotechnology – courtesy of G Bachman, BMBF, Germany.

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	4 Electronics/ Information Technology	5 Automobile/ Mechanical Engineering
	• Write-/Read-Heads (GMR-Effect) • Data Storage layers • Photonic-Components (+GaN) • Vertical CMOS-Elements • Layers for LCD-Orientation • Waver Bonding • Ferroelectric Films • MBE/MOVPE Methods	• Nanotribology • Electrochromic Surfaces • Multilayers
	• Data Storage/Terabit-Chip • Quantum-/Molecular-/Opto-/Vakuum-nano-Electronics (Single Electron Logic, Laser and Light Emitting Diodes, Transistores) • Litography Masks • Structured Write-Read-Heads • Granular GMR-Elements	• Adhesion Avoidance • Injection Systems (with Nanoholes) • Wear and Tear Sensors
)		
	• Photovoltaic Cells • Batteries/Fuel Ceells/Condensators • Conduction Pastes • Resists • Inductive Components • Quantum Components • NLO-Components • Metal Pigments for Data Storage • Mounting and Connection Technology	• Ceramic Automobil Motor Parts • Light-weight Materials • Functional Layers (Antiadhesion-, Climatization-, Anticovering-Layers,...) • Foils and Vanishes with Colour Effects • Gas Storage • Damping Components • Back Lightning • Superhard Alloys
tter)		
	• Wafer Grinding • Wafer Polishing	• Frictionless Bearings • nm-Positioning Technology • Ultraprecision Machines with high Flowrate
	• Structure Analysis • Elemental Distribution (Doting, Compositional and Orbitalcontrast Measurements) • Metrology • Wafer-Inspection • Magnetic Storage Analysis • Control of Layer Growth • Optimization of Signal/Noise Ratio	• Friction Analysis • Roughness • Hardness and Elasticity of Surfaces • Microfabrication in Microscopes with big Volume • Nanosimulation of Material Components

5.4.5. Recommendations

It is recommended that the EU 6th Framework invest substantial funds in the area that is defined as Nanoscience and Nanotechnology. The investment should be of equivalent proportions to that being invested by our major industrial blocks, the U.S. and Japan. This must be of the order of $400 - $500M per annum if Europe is not to be disadvantaged in this technological area that all countries agree will be vitally important to wealth creation in the future. The area of nanotechnology warrants programme in its own right where the programme contents are checked for balance and scientific excellence.

The whole needs to be supported by the correct infrastructure requiring work at all levels and involving everyone from academic organisations through technology transfer institutes and to industry. Binding this together should be a pan-European network to disseminate the results quickly with sub-nets for different topic areas and regional requirements.

This paper outlines the areas of nanomaterials that need to be researched to provide the EU with the technological advantage for future success. The areas of “Extreme” Nanotechnology and biomimetics require vast amounts imagination, intuition and nanoscience research to come to fruition. Its potential is vast and it is proper that the underpinning nanoscience be properly supported. However this should be part of a balanced approach to funding whereby the top down nanoscience and nanotechnology is not overshadowed since the benefits from this area will be considerable in the medium time frame.

It is important to stress that the EU should serve a strategic role by taking the long (>5 year) term view on fundamental research. The shorter term perspective will better and more properly be taken by the growing business community in this area.

The need for more and better modelling is becoming imperative. The more of the basic science that can be achieved via machine “experiments”, the faster the throughput of new molecular combinations for the production of new materials and nanostructures.

It should not be forgotten that this investment will have a major impact on education across the whole of the EU and will provide the skilled workforce that will be necessary to keep the EU at the forefront of this technology race. Coupled with this should be significant public relations programme to keep the citizens of the EU informed of the major benefits of nanotechnology and nanoscience to their lives.

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3. For information on precision engineering and nanotechnology, contact Dr Debbie Corker at EUSPEN – The European Society for Precision Engineering and Nanotechnology: debbie.corker@cranfield.ac.uk and visit its website at http://www.euspen.org/
4. The EU has recently completed an important 'Technology Roadmap for Nanoelectronics' which can be found on the EU's CORDIS website at http://www.cordis.lu/esprit/src/melna-rm.htm
5. Within the EU there is an increasing emphasis on nanotechnology with funding for research and development projects that affect the key objectives of EU policy: quality of life for the ageing population, sustainable development, crime prevention and so on. Individuals with responsibility for co-ordinating nanotechnology R&D in the EU are Bernardus Tubbing: bernardus.tubbing@cec.eu.int and
   Ramon Compano: ramon.compano@cec.eu.int
   A useful German nanotechnology website, http://nanonet.de links to companies and projects Germany wide: likewise the TEKes website has information on nanotechnology activities in Finland, http://www.tekes.fi/
6. For information on nanotechnology in the US visit the NASA website; http://nasa.gov or http://nano.gov and the website of Loyola University, http://www.loyola.ede which has many nanotechnology articles and a comprehensive database on companies, academia and research.
7. There is also a Swiss nanotechnology initiative, TOP21, http://www.ethrat.ch/topnano21/
8. For information on the US National Nanotechnology initiative see http://www.nsf.gov/home/crssprgm/nano/start.htm

5.5. Small-Scale Materials and Structures

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5.5.1. Introduction

"There is plenty of room at the bottom"- the vision of extreme miniaturization, expressed in a celebrated 1959 physics lecture by Nobel laureate Richard Feynman [1], has since then remained an important scientific challenge and guideline for the development of new technologies. A large fraction of modern materials research has been devoted to this goal, but the major benefits of such a micro- and nanostructural design still lie ahead of us.

To realize such objectives, one of the indispensable areas for future research and development is the controlled structuring of materials on all length scales. This applies not only to the precise and accurate shaping of materials to defined external structures but also at the same time to the control of the internal microstructure of the material. This internal microstructure encompasses the granularity of the material and includes materials defects like inclusions, surfaces, internal interfaces, dislocations and microcracks, which in their entirety determine the macroscopic properties of the material. Artificially structuring materials on the nanometre scale or even the atomic scale is of particular interest since "mesoscale" effects occur there which open up entirely new possibilities for applications in (nano)electronics, measuring and sensing [2].

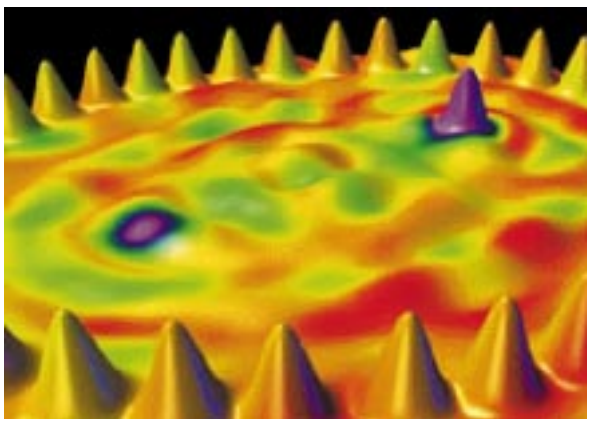

Fig. 5.5. Atomic ring structure displays mesoscopic quantum effects. (Taken from [2]; originally from IBM).

Today materials synthesis is usually characterized by the accidental nature of microstructure formation. Drastically improved materials performance, reliability and reproducibility is expected if the formation of the microstructure can be controlled and adjusted on all length scales. The assembly of complex materials by controlled manipulation on the nanometre scale will make use of advanced lithographic methods but will also include new design principles, such as self-organization by stress fields or (bio)chemical reactions.

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Further advancements in synthesis as well as the ability to tailor-make materials with specific properties critically depends on the ability to model materials microstructure, properties and the processes used for synthesis. Advances in the description of atomic bonding together with the increased computing power have opened the possibility for the simulation of chemical reactors and manufacturing processes which lead to a new degree of prediction of materials structure and performance.

5.5.2. Design of Small-Scale Structures

The performance of today's computer technology was enabled by the down scaling of characteristic feature dimensions of electronic components from a few microns to a few tenth of a micron. This allowed the realization of processors with ever increasing operating frequencies as well as smaller and faster storage components. During the last decade design ideas and fabrication methods from the world of micro electronics have started to inspire other disciplines like the popular field of MEMS (Micro Electro-Mechanical Systems) which led to the creation of miniature sensors (e.g. accelerometers) and micro actuators (e.g. valves, mirrors). Incorporation of such miniature devices into small scale systems will lead to improved performance such as increased power density, improved system reliability through component redundancy and *in situ* monitoring of critical components.

Materials research will be a key element in the realization of new miniaturized devices. The variety of materials which can be processed with micro fabrication techniques is expanding rapidly and ranges from plastics, to metals, and ceramics. New high-performance materials will urgently be required for small engines, micro fuel cells, embedded microsensors and actuators. These may be developed following entirely new engineering design principles, including the use of materials in applications where they could not be used previously. System redundancy may for example allow the use of brittle materials in mechanically loaded systems. Furthermore, such new fabrication methods may also lead to the manufacture of novel materials, e.g. with negative coefficient of thermal expansion or negative Poisson's ratio. It is immediately clear that materials and design issues are intimately connected in the development of micro-components and need to be addressed together. This will require the cooperation of materials and mechanical engineers, even to a greater degree than in today's development of large-scale components.

5.5.3. Interfaces and Composite Materials

For ever smaller structures, surfaces and interfaces gain in importance as the surface-to-volume ratio increases. We need to develop, therefore, greater understanding of the relation between structure, thermodynamics and properties (diffusivity, reactivity, segregation behaviour, equilibration conditions) of surfaces and interfaces. Surfaces and interfaces obviously dominate adhesive and frictional properties of small scale materials. In particular, they also affect the plastic response of a material and the brittle or ductile behaviour. Artificially layering compounds with different properties or different internal stresses will allow circumvention of classical trade-offs and lead to new materials with unprecedented combinations of strength and toughness, conductivity and hardness or magnetic and mechanical strength.

A common weakness of small structures is their limited thermal stability. The reason lies in the fact that kinetic materials processes are size-dependent on a variety of scales. Examples are the equilibration of surface and interface shapes, the interfacial reactions (including the formation of non-equilibrium phases), and the formation of mesoscopic interface structures such as ledges. Assessing thermal stability of metastable structures requires detailed understanding of the interfaces involved in nucleation processes.. The main unknown is the energy of the interface between a second phase nucleus and the matrix. Determining this energy is particularly challenging in the case of nucleation from a liquid, since the interface is difficult to access experimentally, and modelling of its structure and thermodynamic properties is complex. However, the small size and the low stability of very small structural elements opens the possibility to use self-assembly and similar methods for structuring, which rely on small driving forces.

Organic thin films are in many ways different from metallic or ceramic ones. By constraining a polymer to a thin film, its conformation can be quite different from that in the bulk. Organic monolayers, often self-assembled, either on a substrate or as a membrane, have unique structure, thermodynamics and mechanical and functional response. They can also be used to coat small particles and thin films to induce functionalisation and self-assembly. Research along these extremely promising lines is only in its infancy.

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5.5.4. Interface to Biological Materials

Lessons from biology can fertilize materials research in many different ways. Three billion years of evolution paced by stress ("Survival of the fittest") has produced a number of remarkably efficient materials and molecular devices (photosynthetic centre, efficient molecular motors, controllable molecular channels). The use of such molecules in assembling inorganic matter into functional materials could potentially revolutionize materials synthesis.

For example, spontaneous organization is an almost universal feature of complex biomolecules that renders them ideal for fabrication, provided we can engineer them to our needs. By an appropriate choice of functional end-groups of the self-assembled monolayers intelligent substrate surfaces could be created allowing selective bonding between many different materials. Tiny particles of insulators, semiconductors and metals can be organized into functional materials, a process that produces materials from the "bottom up" rather than from the "top-down". No lithography will be needed to realize specific mesoscopic structures and it can be foreseen that self-organizing concepts will be used for fabrication in different ways.

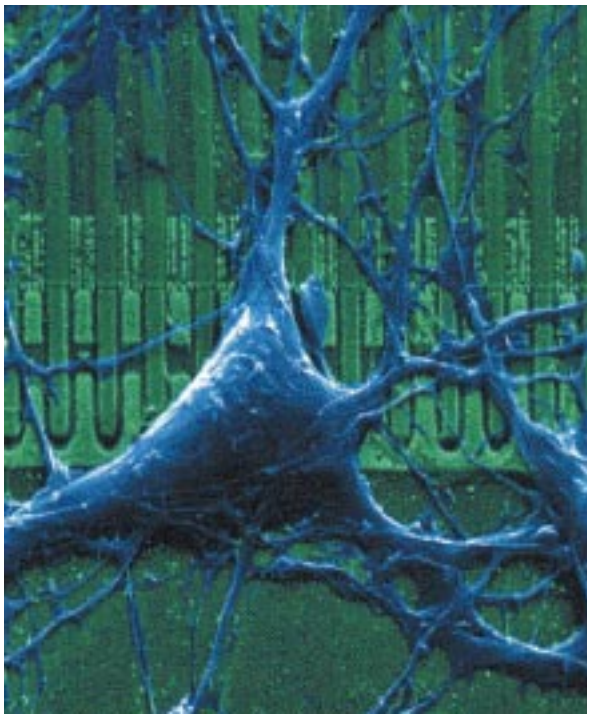

Fig. 5.6. Neuron on an oxide-covered silicon chip. (From Ref. [3]).

Nature can also inspire materials research in the creation of optimized interfaces and surfaces. In a rather counter-intuitive way, finely structured shark skin was found to exhibit better hydrodynamic behaviour than perfectly polished surfaces. Similar surprises happened in the search for non-wetting surfaces ("Lotus flower effect"). In the field of microtribology, optimally structured surfaces were found in insects which could guide the development of microstructured reversible adhesive contacts.

In small-scale materials the internal and external structure sizes overlap with the biological scales which in principle allows more detailed studies of the intimate contact between inorganic structures (machines) and living organisms or cells (see Fig. 5.6) reaching as far as exchanging information across such contacts [3]. Better control of these interfaces will change our possibilities for activating or passivating surfaces for the contact to living organisms and may open new ways for medical treatment. However, this will require much more intense collaboration between biological and materials research which will very likely produce exciting materials innovations in the future.

5.5.5 Understanding Materials Across the Scales

An important issue in materials science is how mechanical properties such as strength, hardness and toughness, magnetic or electrical properties scale with the characteristic size of a structure. This issue is especially important for materials problems in micro- and nano-technology. Computer modelling has become an indispensable instrument for the advancement of the theoretical understanding of materials, particularly for small scale materials and systems, where the magnetic, electronic or mechanical properties directly depend on the internal (microstructure) and external (shape) structure. Particular attention has recently been directed towards the question whether and how the properties of a functional system can be predicted on the basis of its known atomic or molecular composition. This depends critically on the understanding how a particular crystal defect or a particular molecule contributes to the collective materials properties and the function of the system. The simulation or prediction of such effects requires the connection of different modelling schemes on significantly different length and time scales. Many fundamental aspects of such a connection remain to be explored, particularly for the connection between discrete (atomistic) and continuous models.

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Experimentation and simulation are equally important to advance the understanding at this transition between different scales and different phenomena. Particularly *in situ* experiments geared towards testing modelling predictions will be of greatest need. This need is generated firstly by the fact that the small scale structures are usually metastable structures, far away from equilibrium where transient behaviour is of outstanding importance. Secondly, the modelling of scale transitions usually involves multiple phenomena which can not be separated and therefore have to be compared directly to (*in situ*) observations. The combination of in-situ experimentation and simulation will be particularly fruitful in understanding nucleation and interaction of crystal defects which are the basis for the theoretical modelling of the mechanical properties, plasticity, fracture and fatigue of small scale materials. Similarly, recent advances in micro-focus X-ray diffraction or *in situ* microscopy techniques enable materials synthesis or deposition processes to be studied; this will allow validation of computer simulations of the microstructure formation, of nucleation and growth phenomena. Considerable research effort is, however, required to reach these ambitious goals.

5.5.6. International Situation and Current Needs in Europe

The international situation in the research on small-scale materials and particularly on nanotechnology has changed significantly over the past few years. It was characterized by almost equal strength and similar amounts of government expenditures in the U.S., Japan and Europe [4]. Europe was among the world leaders mainly in analytical methods, lateral nanostructuring and ultraprecision engineering. Funding has been increasing moderately. The main funding sources are the 5th Framework Programme of the EU and national nanotechnology programmes like the German BMBF-initiative “Nanotechnologie”. The particular strength of Japanese research is in quantum functional devices and (nano)biotechnology. Nanotechnology research in Japan also benefits from a very strong industrial research effort with many close collaborations between industrial research centres (Hitachi, NEC, Toshiba,..) and academic or other government funded research. In the U.S. the entire small-scale materials sector got a huge boost through the National Nanotechnology Initiative which effectively tripled government expenditure on nanotechnology within the last 3 years (to about 0.5 billion Euro in 2001 [2]). This enormous drive towards nanotechnology gave U.S. research a very significant competitive advantage not only in funding but also in public awareness in identifying nanotechnology as a key intellectual and economical subject of the future.

Current weaknesses in Europe are: a lack of a unifying view on small-scale materials and systems including their manufacturing, analysis and their performance through the entire life cycle, a lack of intellectual drive towards materials science in general and a lack of cross-disciplinary collaboration in the research for new small-scale systems. Furthermore there is also a lack of entrepreneurship in connection with and around the research programmes particularly in comparison with the situation in the U.S. All these weaknesses would vastly benefit from a large-scale concerted action towards materials research for which the research on small-scale materials is a spearhead.

5.5.7. Conclusions

The field of small-scale materials and structures is particularly promising for creating scientific and technological breakthroughs and innovations. Studies of size-effects on the behaviour of materials and the functionality of systems are at present only in their infancy and will require substantial research efforts. Of paramount importance will be an integration of manufacturing control, the simulation and the specific adjustment of the properties and the prediction of their development during the service life of the systems. Further progress in this area will critically depend on close collaborations of materials scientists with physicists and mechanical engineers, on the one hand, and bioscientists, on the other.

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5.6. Colloid Physics and Chemistry

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5.6.1. Introduction

Colloid chemistry and physics is the science of making, characterizing, and examining the properties of objects or matter structured on the length scale of some nanometres. The relation to modern notations such as "nanotechnology", self-organization into ordered "nanostructures", "nanocomposites", or "nanoparticles" is obvious, and colloid science is the scientific base of a whole range of applications in modern technologies.

An important differentiation to be made is that not all parts of nanotechnology are based on colloids, since colloid science historically focuses on solution or wet chemical precursors, but does not consider gas phase procedures or solid state approaches towards nanostructured elements. In colloid science, there is also a certain dominance of soft materials (polymers, surfactants, supramolecular units, bio-matter), but components made of metal, semiconductors, or ceramics are also quite frequently used. It is just that the approaches in classic semiconductor science or solid state physics are clearly different from the approaches used in colloid science.

5.6.2. Status of the Field and Deficiencies in Europe

The field has experienced large sophistication (and an unparalleled scientific renaissance) within the last 10 years, and major scientific trends arising from colloid and interface science were for instance nanoparticle research, self-assembled monolayers, ultrathin organic layers, as well as the development of casting and template techniques. The breakthroughs also arose from development of modern analytical techniques like scanning probe microscopies, neutron-, X-ray-, and light scattering that were able to describe the objects of interest, bridging the dimensional gap between the macroscopic, solid state world and the former chemistry of molecules. Those recently grown fields will continue to drive the development of new materials, but the colloid science in itself and the needs of other disciplines will create a number of new light signals where colloid science might go to.

One of the most visible political decisions of the last years was the "National Nanotechnology Initiative" of the NSF [1], which put 422 million $ into nano-sensitive infrastructure, and a significant part of it in the above mentioned fields ; this corresponds to a total budget increase of 56 %. Corresponding European programmes are still missing such that there is serious chance of loosing the race for the best heads and the best innovations in this very promising field between Asia, Europe, and America. This is why joint efforts in previous and current strongholds in this area are to be kept or to be established, and must receive better support.

5.6.3. Future Visions

In the following, we will list from our personal viewpoint some selected breakthrough fields where we expect major developments with either strong scientific impact or benefits for the society.

(a) Nanocomposites for engineering purposes

The hybridization of organic and inorganic matter on the nanometre scale, e.g. polymers and inorganic or metallic nanoparticles, will add a new class of materials in between polymers and ceramics [2,3] It is expected that those materials show the easiness of processability of polymers, but inherit some of the properties, e.g. scratch resistance or magnetism, of the inorganic side, too. Scratch free plastic car windows (for light-weight construction), light-weight eye glasses, highly resistant coatings and paints for machines and furniture, carbon nanotube reinforced thermoplasts (improves mechanical stability, conductivity, and enables recycling), or the fuel saving "green tire" are just some examples for nanocomposites to be made with the clear potential to impact technology and society.

(b) The interface between the bio-world and materials

The coexistence of biological objects, such as cells, and technical devices, e.g. in biosensors, for artificial senses, in prostheses, for artificial organs and in tissue engineering will continue to demand a set of instruments for an "interfacing" between the two worlds. The notation "interfacing" contains elements of the physicochemical interface, that is the adaptation of chemical functionality, conductivity or elasticity, but also elements of informatics, that is the possibility and encoding of information transfer throughout the boundary between biological and artificial world [4].

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Molecular or colloidal "chimeras" such as polymers with biological parts and synthetic blocks are starting to be developed in tissue engineering [5] and are regarded as first steps towards "amphiphiles" (= both loving) for this special problem.

(c) Biomimetic material science

The superb performance of biological material such as bone, seashells, wood, tendon, hair, or spiders´ silk is due to a hierarchical superstructure of the materials where structure control is exerted at every level of hierarchy [6,7] In addition, it must be pointed out that those materials are created around room temperature, represent in many cases optimal cases of lightweight design, are made of simple components such as calciumcarbonate or polypeptides, and are recyclable and sustainable.

Procedures have to be developed which allow material scientists a similar control over materials structure on all length scales, presumable by combination of traditional procedures with new nanometre- and micrometre specific techniques, such as template procedures, controlled crystallization/growth or directed nucleation of foams [8].

(d) Functional thin organic/polymer layers

The further development of thin organic layers onto other materials is currently mainly performed for either protection against corrosion or lubrication. The physical/chemical design of more sophisticated functional interfaces will create another dimension of possibilities for material science. Examples for that are coatings with ultralow-surface tension (dirt repellent, tribology), surfaces with the ability to reconstitute misfolded proteins, or surfaces which assist the formation of biofilms (materials coated by wanted bacteria or algae) [9].

(e) Catalysts with a rational nanostructure

The increase of the efficiency of large scale chemical and engineering processes, e.g. oil refinement, the redirection of product streams or fuel cell technology relies mainly on the development of new catalysts and catalytic procedures. The methanol reforming process (the generation of hydrogen from methanol) for fuel cells or a potential efficient refining of the 20 wt% heavy crude oil fraction are just two examples where the advantages for a balanced technological development are very obvious. Although there are concepts for such catalysts, their realization relies on a better understanding of the catalytic process as well as the ability for a rational design of those structures with characteristic structural details that are necessarily on the nanoscale and beyond the tools of classical chemistry.

(f) Colloidal diagnostics and drug carriers

In pharmacy, there is an ongoing trend to go from "molecular" drugs to the development of vectors or complete systems where the drug or molecule of action is equipped with a transport and protection system and a "homing" device to make the drug more efficient and to allow applications usually not possible for the drug itself (e.g. inhalation or transdermal application of insulin instead of injection) [10,11].

It is common sense that those active systems are carefully designed and composed colloidal entities, where each of the components fulfils a special task. Similar arguments hold true for simple, multipurpose diagnostic kids (or detection kids) for the rapid ex-vivo analysis of diseases, infections, and intoxication of food and water.

(g) Colloids with gradients and broken symmetry: directional forces and differentiated 3d-self assembly

Previous work on self assembly has shown that the complexity of the resulting superstructures is restricted to rather simple shapes, which is due to the high symmetry of the starting objects and the connected interaction fields. It is therefore a current task to create building blocks with broken symmetry such as "Janus spheres" or "Janus coins" are objects with non-centrosymmetric fields which can line up in more interesting (and useful) superstructures, as they are for instance found in living nature. This would allow self-assembly to go "around-the-corner". This topic is closely related to "biomimetic materials" and the question of structural hierarchies in artificial materials.

(h) Complex colloidal entities with function: "nanofactories" and "artificial cells"

Recent developments on encapsulation technologies allow creation of closed hollow objects from polymers or polyelectrolytes in the micron size range, where functionalities such as ion channels, photoactive sites, proton separation, or chemical gradients can be easily implemented [12,13]. These entities are called "cells" (used in the general semantic notation). Such "artificial cells" or "nanofactories" have the chance to become the most complex artificial objects on the molecular scale which can be released with a function, e.g. harvest solar energy, actively collect heavy metal ions, or release chemicals at outer programmed stimuli.

(i) New principles for chemistry: compartimentalization and single molecule chemistry

Beside direct applications, colloid science of the next years also has to consider new "instruments" to be brought into material synthesis. One graphic example for those is the concept of compartimentalization or single molecule chemistry [16]. Compartimentalization is the (biomimet-

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ic) principle to isolate molecules from each other and to perform complex chemical reactions or folding/crystallization procedures. Such a reaction is expected to occur in the compartimentalized state in a purely intramolecular fashion and obey a higher degree of control. This is important for molecules with more than one reaction site or many possible reaction pathways. Since the processes are done on single molecules, but in a highly parallel fashion (many compartments), the mass flux is still of significant size. Obviously, this principle is already used throughout biosynthesis, but not applied for artificial systems.

5.6.4. Conclusion and Recommendations

It is not only our, but also the opinion of many technology agencies that colloid and interface science is one of the real opportunities to combine a sustainable and environmentally friendly development with the forthcoming technological needs of our society [15]. Even more important, some long term goals (like the preservation of the climate, fuel cell technology, energy neutral living areas, low energy consumption mobility) cannot be reached with the standard technology, and colloid and interface science plays a key role in all solution strategies.

Beside of the scientific possibilities and the long term needs of society, this type of technology has already grown to a major market, and a conservative estimate of the market volume for 2001 has lead to a sum of 100 billion DM [16].

Considering this potential importance, it is obvious that the chances for society and the current public funding of the topic have no relation. Even the 2.5 % of net cash flow which are typical for a G7 country to preserve active research and development in a field are well above any public science programme in this field. It is worth repeating that both the American and the Japanese science systems already have reacted and started to support this field as one of the future key breakthrough fields of science policy, both financially and by adequate organizational support.

The European science system is just a the beginning of an adequate reaction, mainly still on the base of small test programmes or feasibility analyses. We recommend a fast and substantial reaction, potentially focussed to the specific demands of society (e.g. by the establishment of virtual, interdisciplinary European Institutes covering topics such as “Artificial Cellular Nanofactories”, “Catalysis 2010”, “Biomimetic Materials”, or “Energy neutral villages”), where colloid science will certainly contribute. In addition, the organization principles and the reaction times of the science support system have to be significantly de-bureaucratized and shortened.

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5.7. Mechanical Properties of Metals and Composites

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5.7.1. Introduction

Topics such as elastic properties of materials, fracture toughness, fatigue crack propagation, plastic yielding at room temperature, at elevated temperatures, creep, viscous flow etc. all belong to the concept of "Mechanical Properties".

Furthermore, several metal families are involved, of which the main ones are those based on steel, on aluminium, on copper, on titanium and on magnesium. The number of researchers working in all these fields, and the number of industries involved, is vast. In this text, focus will be mainly on metals and on plastic properties at room temperature, including strength and ductility. Even then the variety of activities, needs and potentialities is great . The present discussion is written with an eye to the future, and will therefore take the future needs of society as its starting point, rather than the present state of the art.

5.7.2. Future Needs of Society Regarding Materials for Structural Applications

(a) Weight and energy saving

By "structural applications" we understand all applications for which the main function of the material is to carry a load. In the transport sector (cars, trucks, trains, aircraft), weight savings will become increasingly important, because they are intricately connected to energy savings by reduction of fuel consumption. But there are other sectors as well for which weight savings are important. For examples, by using lighter but stronger materials, it may be possible to make bridges wider without having to replace the foundations. Not surprisingly, the most stringent demands for weight reductions come from expensive products, such as sporting goods for top-level sports, and of course aerospace.

In the decade to come, car body parts from mild steel will partly be replaced by aluminium alloys, which on their turn may be replaced later by special high-strength magnesium alloys. Reinforcement parts from mild steel are already being replaced by parts from high-strength steels, allowing considerable weight savings.

The second decade to come will see further weight reductions by the replacement of some steel parts by carbon-fibre reinforced plastic (composite material) or by aluminium-based metal matrix composites. Parts from high-strength steel may be replaced by high-strength titanium alloys. Finally many parts from carbon steel will be replaced by stainless steel, which not only lasts longer but also has a higher strength.

In the hulls of recent military aircraft, the share of aluminium is reduced to as less as 16% and steel to 6%. They have been replaced by advanced Ti-alloys and by polymer-based composite materials. In the civilian aircraft industry, evolution is much less drastic although the evolution is the same.

(b) Micro- and "nano"-technology

The importance of structures and devices with sizes in the micrometre-range such as interconnects, microvalves, microswitches, often also deposited on Si substrates, will become more important in the future. (This field is often reckoned to belong the "nanotechnology" field, although its scale obviously is that of micrometres). State of the art is that it is now possible to make such structures or devices. Optimization of properties has just begun. More focus will have to be given in future to the mechanical behaviour of these structures or devices. In interconnects for example (material: copper or aluminium), the lifetime and functionality are greatly affected by the residual stresses present. The latter depend on the processing of the component, but also on the material properties of the interconnect, such as elastic constants, and especially the lattice misorientations at grain boundaries. The study of this requires advanced electron-microscopical techniques which allow for the simultaneous acquisition of topological and crystal texture data, combined with advanced material models such as crystal-level elasto-plastic finite element codes. In micromachines (material: often silicon), the grain boundaries are equally important, as they are potential sources of stress concentration possibly leading to premature failure of the device.

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5.7.3. State of the Art and Research Needs

(a) Steels

Fig. 5.7 shows the combinations of strength/ductility which are available today for steel sheet for car bodies. The two material families at the right (TRIP, high-strength Dual Phase) are still under development. Such steels are very complex; they contain several phases; the ductility is enhanced by special effects which strongly increase work hardening, such as transformation-induced plasticity. Fundamental research is needed in order to obtain even better materials, for which the bands are shifted either to the top or to the right. These materials will probably be multiphase materials as well, or materials with a nanostructure, or a combination of both. For example, it is conceivable to develop pearlitic steels with interlamellar distances in the lower nanometre range, which will probably have superior properties due to the effect of the lamellar structure on both strength and work hardening. Other types of steels which would also exploit the "lamellar effect" are also conceivable. A discussion on the scientific issues related to multiphase alloys is given below.

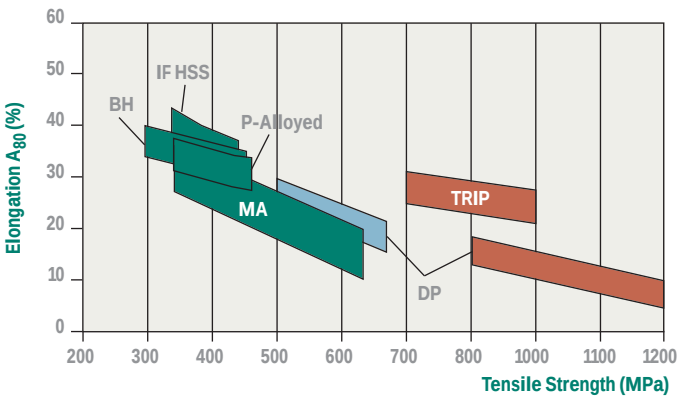

Fig. 5.7. Combinations of strength and ductility (elongation) for various steel families.

(b) Aluminium alloys

The art of using several alloying elements in order to obtain much higher strength in aluminium alloys is well developed. One of the most interesting ways to achieve this is by precipitation hardening. This "art" is now evolving to become a "science" by doing extensive studies on these precipitates, their crystal structure, the degree of their coherence with the matrix, their stability. This research will lead in the decade to come to further substantial improvements of these alloys. One of the questions to be addressed is the study of the stability of age-hardened alloys (an application of precipitation hardening) at temperatures in the range of 150°C - 200 °C. High-strength aluminium alloys which would be stable in that range would allow for important weight and energy savings in aerospace applications.

Many advanced aluminium alloys are also multiphase alloys. See the discussion on multiphase alloys below.
For the rest, more work has to be done on developing reliable constitutive models to be used in design applications. For some alloy systems, wide-range models exist for work hardening as a function of strain rate and temperature [1], but not for all alloy systems. Moreover, the existing model, how complex it may appear [1], should still be extended to include anisotropy and strain path effects.

(c) Titanium alloys

Aerospace industry has developed some truly high-strength Ti-based alloys with very interesting microstructures (some of them lamellar). Some of these developments are unfortunately not in the public domain (military secrets). Companies which build both military and civilian aircraft can of course apply these alloys also in civilian application, which cannot be done by companies which only build civilian aircraft. From a more scientific point of view, many issues remain unresolved, again because not enough is know of the behaviour of multiphase materials at the micro-to nanometre scale. (See the discussion on multiphase materials).

(d) Copper alloys

The knowledge acquired for other metals (see above) would be used to develop copper alloys which combine a high electrical or thermal conductivity with a high strength, which might have very important technological applications.

(e) Composites

Composite materials, either based on a polymer-matrix or on a metal matrix, and reinforced by fibres have a high potential to develop materials with an extremely favourable ratio between strength and weight. The state of the art is there that these materials can be produced, but that processing still needs a lot of work to improve. The true understanding of the mechanical properties is now emerging, but still has to be done in many cases. Again they will very much depend on the interaction between phases, development of stresses, and of course on the understanding of the behaviour of the phases themselves. In view of the high potential of these materials, a strong effort for further fundamental research to raise it to the same scientific level as the research on metals, is imperative.

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5.7.4. Scientific Trends

(a) Multiphase and nano-structured materials

Before the material scientists at steel companies, aluminium companies etc. can really design new materials which derive a high strength from either a multiphase structure or a nanostructure, the institutions for fundamental materials research must provide answers to a certain number of questions. A few examples:

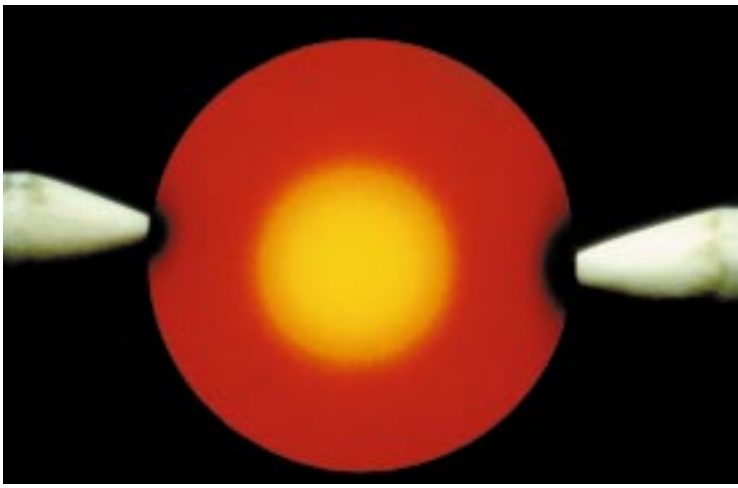
- By which dislocation mechanisms is work hardening achieved in the individual phases of multiphase materials?
- What are the relations between morphology (e.g. lamella orientations) and crystallography at the time that the microstructure is first formed?
- How do the phases interact with each other during plastic deformation?
- To what extent is the work hardening pressure dependent? (it might be relevant in cases for which phase transformations may contribute to plastic deformation)
- Down to which grain size/interlamellar distance would dislocation glide remain the dominant mechanism of plastic deformation? By what is it replaced in the very low nanometre range? How does this affect work hardening and resistance against crack propagation?
- What are the glide systems in phases like cementite, bainite, martensite? What is the values of the critical resolved shear stresses?
- Why can the fracture of cementite upon plastic deformation apparently be avoided in certain materials?
- Which phase stresses develop in the various phases, how can they be measured, how can they be modelled? How do they affect ductility and strength?
- How is the thermodynamic equilibrium of the various phases (some of them metastable) affected by the presence of high stresses and high dislocation densities after plastic deformation? (important question as to the stability in time of properties of a material strengthened by work hardening).

(This list is not exhaustive). To be able to answer these questions, advanced experimental techniques have to be developed, difficult measurements have to be carried out, and the best "tools" of fundamental material physics need to be used. Some questions will require the use of molecular dynamics-type approaches, or, on a slightly more coarse scale, dislocation dynamics. Scale transition schemes will have to be used to translate the conclusions into workable models for design applications (see below).

(b) Atomistic modelling

A promising path is the use of atomistic modelling/molecular dynamics for the study of mechanical properties. Studies are being done on

- the behaviour of dislocations in a crystal;
- the propagation of a crack in a crystal;
- the plastic deformation of nanostructured polycrystalline material, when the grain size becomes so small that dislocation glide no longer is the microscopic deformation mechanisms.



Laser induced thermal shock measurement: influence of extreme material loading by temperature changes are simulated.

(c) Dislocation dynamics

At a somewhat higher scale (106 atoms), one studies the behaviour of several hundreds dislocations by using specific models for the behaviour of a dislocation in a crystal lattice. This might some day lead to a full understanding of the dislocation patterns which are observed in deformed materials.

(d) Multiscale modelling

A successful model at atomistic scale cannot really be used for engineering applications. Schemes based on scientific principles have to be developed to derive a model which can be used at a particular length scale from a model developed from a lower length scale. The transition form the atomistic level to the dislocation level, then to the subgrain level, then to the grain level, finally to the macroscopic level will be achieved in this way during the decade to come.

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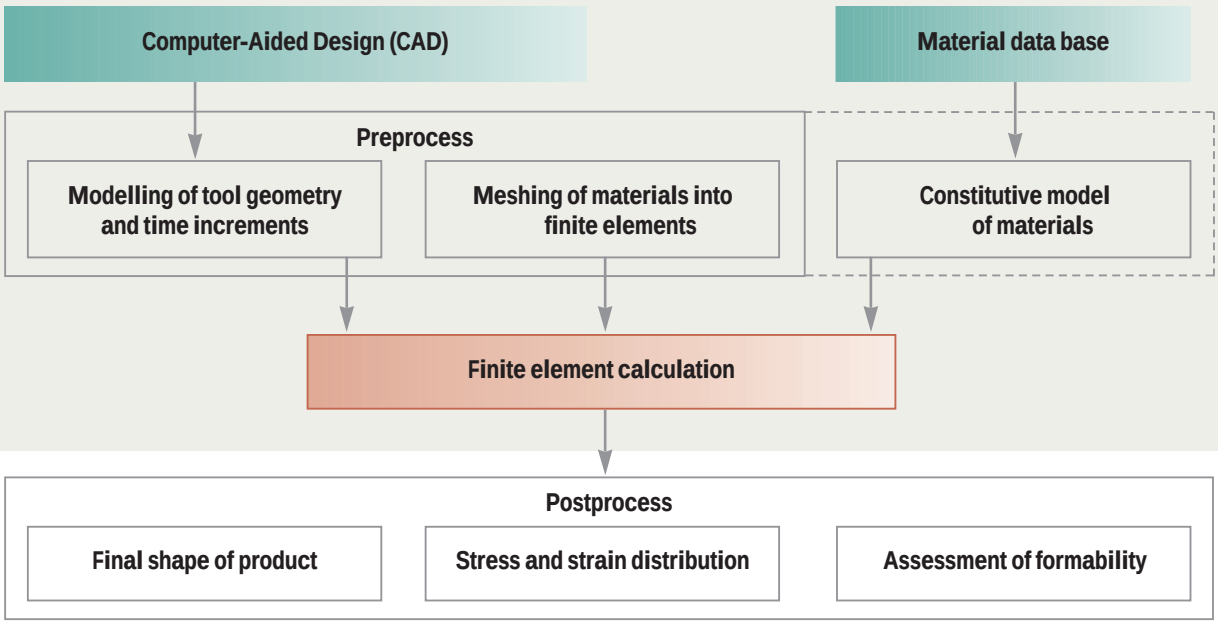

Fig. 5.8. Scheme of an FE-software system which can be used to design deep drawing products.

5.7.5. Application of Modelling in Design of Components

Advanced high-strength/light weight materials will not be used to reduce weight in cars and other systems unless design procedures in industries are adapted. This is illustrated by the following example. Suppose that a pressed part of a car (for example, a reinforcement column used for better protection of the passengers) is normally made from low-carbon steel. By making it from an advanced aluminium alloy or a high-strength steel, one can reduce the thickness of the plate while maintaining the same strength before fracture. But this would strongly reduce the elastic bending stiffness (this issue has nothing to do with fracture!) if the design is not adapted for the rest. However, it is possible to obtain a sufficient bending stiffness by adequately adapting the design. Only, the designers of industry are not familiar with this. Their design principles have been optimized by decades of experience with low carbon steel. Unfortunately, there is no time left to acquire experience in the same way with the new advanced lightweight materials. The answer of materials scientists and research managers to this problem is to modernize the design process by incorporating reliable constitutive models for the materials behaviour into finite element models for the mechanical behaviour of components. This makes it possible to optimize a product and the production process needed for it by means of computer-aided design and computer-aided manufacturing, thereby essentially gaining one or two decades in the introduction of advanced lightweight materials in industrial applications.

Fig. 5.8 illustrates the role of the constitutive model for the mechanical behaviour of the materials in such system. The state of the art is as follows:

- advanced material models which can realistically describe the mechanical behaviour of single-phase polycrystalline materials (steel, aluminium alloys, copper alloys, α-Ti alloys or β-Ti alloys) including important aspects such as texture-based anisotropy and work hardening (also at changing strain paths) are under development at present.

- in the decade to come, it is expected that this work will be extended to advanced multiphase materials. That means that all the knowledge acquired by studying the physical problems listed above (see for example the section on multiphase and nano-structured materials) needs to be brought to a level of quality where it can be implemented in quantitative models. Models of this quality level will hopefully be transferred from the laboratories of universities and research institutions to the industry during the second decade of the 21st century.

- implementation of advanced non linear model like these into FE-codes is a formidable problem by itself. Existing codes tend to become unstable if realistic materials models are used. To solve this problem, the best that theoretical mechanics can offer is needed. Several leading groups in the field of FE modelling are now working at this.

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5.7.6. Advance of the United States as compared to Europe

A detailed analysis of this issue for all the topics listed above would require a much longer document. So only the most striking aspects will be given.

The Unites States certainly has an important advantage in the following fields:

- Study of advanced Al- and Ti-alloys and composite materials. Any institution or company working simultaneously on military and civilian applications, and hence having access to "military" results for civilian applications, has a great advantage.

- Implementation of advanced material models in FE-codes. This work too is strongly supported by the needs of military and nuclear industry.

- "Micro" and "Nano"-technology. The United States are currently doing a great research effort, also in the subfield of "microstructural applications".

References

There is no single review paper covering all the topics listed above. A complete literature list would be many pages long. So only a few references will be given, to allow for an estimate of the complexity of the issues depicted in the present contribution.
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About advanced FE modelling of polycrystalline materials (work of Paul Dawson et al., Cornell University, Ithaca, N.Y., USA):
2. P.R. Dawson and A.J. Beaudoin, "Finite element simulation of metal forming", in "Texture and Anisotropy. Preferred Orientations in Polycrystals and their Effect on Material Properties," Kocks, U.F., Tomé, C.N., Wenk, H.-R., Eds., . Cambridge University Press, Cambridge, U.K. (1998) 533-560.

5.8. Electronic Structure and Correlation

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5.8.1. Present Status

Basic research in materials science includes the study of electronic structure as the basis for all properties of materials employed in applications. Examples are electrical properties, magnetism, optical properties, the crystal structure, etc. Therefore, the study of microscopic electronic properties complements investigations of macroscopic quantities, which often are aimed directly at improving specific properties of materials utilized in applications. Also, the goal of understanding materials properties comprehensively by applying variable scale modelling requires input about electronic structure.

Materials whose specific features of the microscopic electronic structure are employed directly in applications are semiconductors, superconductors, and magnetic materials. But the electronic structure is also the root of almost any other material property, e.g. the extraordinary mechanical properties of some carbides and nitrides, optical properties, catalytic activity, etc. Therefore, the study of electronic structure both by experimental and theoretical investigations will be of central importance for exploring basic phenomena, which may lead to novel applications.

For the study of electronic structure, there is a broad range of highly developed spectroscopic methods available. The most direct probe of electronic structure is photoemission. This is complemented by techniques such as photoabsorption, linear and non-linear optical spectroscopy, inverse photoemission, etc. Also on the theoretical side considerable progress has been achieved over the last years. This includes a higher degree of reliability and precision with respect to the ground state electronic structure, not only for simple systems, but also for ever more complex materials. Also, the spectroscopic properties, which inevitably involve excited states, can be described so that in many cases very good agreement is achieved between experiment and theory.

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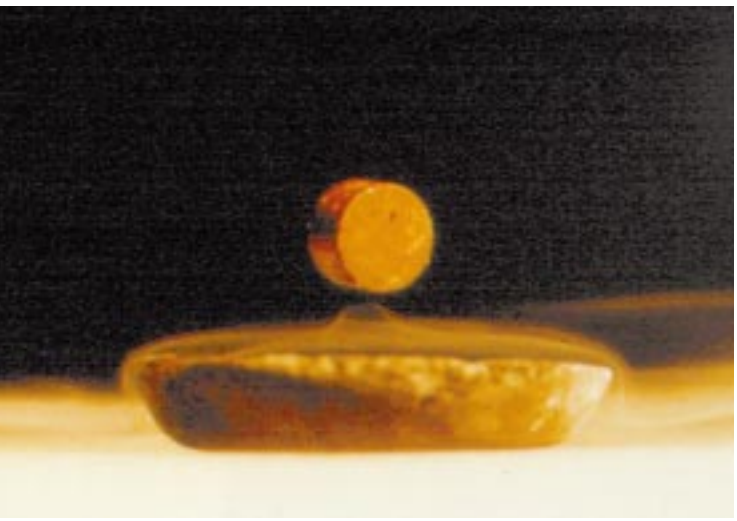
5.8.2. Magnetism

Although the *d* electrons of transition metals are clearly itinerant, they show in many experiments features of localized moments. These two aspects are only starting to be adequately addressed by introducing realistic models for self-energy effects etc. Magnetic anisotropy, a key parameter for employing magnetic materials in applications, can be calculated for metallic systems in the bulk. However, in many applications surface anisotropies play a crucial role, so that this capability is being extended to thin films and surfaces, taking the interaction with substrates or neighbouring films in multilayers into account.

Magnetic semiconductors, which can be formed by doping or alloying semiconductors with suitable transition metal ions (e.g. Mn to form GaMnAs), have potential applications in spin electronics, as they provide a simple way to combine spin dependent phenomena with conventional semiconductor operation. Therefore, the study and development of such materials is being vigorously pursued in the Japan and the U.S. The origin of ferromagnetic order in systems with low carrier densities and low concentration of magnetic ions, found both in semiconducting and metallic systems, is presently investigated in many laboratories.



Levitation of a cylindrical magnet above a high-temperature YBa_2CuO_3 superconductor disk cooled to liquid nitrogen (77 K) temperature.

For applications in data storage, the speed of magnetisation reversal is a crucial parameter. Therefore it is of interest to determine the limit for such a process and to possibly explore ways to move the limit to faster rates. In this context, the influence of reduced dimension and finite sizes is also of outstanding importance. Dynamic phenomena are being studied by pump-probe experiments using pulsed lasers.

Computer technology in the future will probably employ novel devices based on spin dependent transport of carriers. The background is that reduced sizes of structures lead to increased scattering, posing a limit to scaling down the size of the structures in integrated circuits. It is expected that such scattering processes will not affect the electron spin. This suggests that devices based on spin-dependent transport may be scaled down to smaller dimensions than conventional electronics. The materials science issues for this goal concern the efficient injection of polarized carriers into the devices, the investigation of the spin dependent scattering, which may result in a loss of the spin information, and the development of active devices (“spin transistors”). Sensors based on spin dependent transport are already mass-produced as reading heads for disc drives, and their use is expected to increase strongly. The development of non-volatile memories employing spin dependent transport, which is presently taking place, will lead to an important technology with widespread applications.

For magnetic as well as for many other classes of materials, the understanding and possible modification of mesoscopic phenomena is one of the keys for future technologies. As the magnetic units, which contain one bit, become ever smaller, the size of these elements will eventually fall below the superparamagnetic limit. This leads to the goal of reaching a better understanding of the properties, which govern this limit, primarily the magnetic anisotropy, in order to tailor or modify them, e.g. by alloying, and/or via the shape of the elements.

All the studies discussed here depend on high quality preparation of ultrathin magnetic films and multilayers, including lateral structuring on the nanometre scale, and characterization by complementary techniques as discussed in the other sections of this booklet.

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5.8.3. Highly Correlated Systems

Electronic correlations in solid materials lead to a narrowing of electronic bands. If the electronic structure is influenced by correlations, bandwidths measured e.g. by photoemission are smaller than calculated by standard techniques (e.g. local density functional theory). In materials with strong electronic correlations the properties of the itinerant electrons can often be described in terms of a Fermi liquid where the excitations of the itinerant electron system, termed quasiparticles, have a one-to-one correspondence to those of the non-interacting electron gas. These quasiparticles carry a renormalized effective mass, which is usually significantly larger than the mass of the free electron. The residual interactions among the quasiparticles are modelled by additional parameters.

In materials with localized 4*f* or 5*f* moments, the exchange interaction between the localized moments and the mostly *d*-like conduction electrons leads to an indirect exchange interaction between the localized moments on different sites, in most cases favouring antiferromagnetic order. If the interaction is sufficiently strong, a local singlet (Kondo singlet) may arise. These local singlets behave as extremely heavy quasiparticles.

The competition between the Kondo and RKKY interactions governs the behaviour of these materials. The superconductivity, which appears in a number of these systems, appears to be mediated by antiferromagnetic correlations rather than by phonons. The magnetic moments associated with the AF correlations are extremely small, of the order of 0.01 μ_B.

The interplay between superconductivity and magnetism is a key feature of high temperature cuprate superconductors. Whereas the symmetry of the order parameter has been established, a number of questions remain unanswered. An important issue is whether spatial correlations of charge carriers (so-called stripes) do exist and what role they play for superconductivity. Also, the origin of the many unusual properties in the normal state of the cuprates is not fully understood. An example is the "smeared" energy gap ('pseudo gap') appearing in many properties.

The manganites are structurally related to the cuprate superconductors, both belonging to the class of Perovskite structures. Although known for a long time, these materials are now being studied intensively because of the high potential for applications arising from the so-called colossal magnetoresistance (CMR) effect. In these materials the interplay between magnetic, charge and orbital ordering governs the physical properties. Transition metal oxides offer the possibility to modify the physical properties over wide ranges by synthesising materials in which the oxygen ions – instead of forming complete planes – assemble in smaller units, e.g. chains, ladders, or more complicated parquet patterns.

5.8.4. Theory

Because of the increasing complexity of materials for future applications, theoretical research will play a vital role in the context of material science. In particular, the influence of electronic correlations can only be addressed by joint efforts of theoretical and experimental investigations.

A major contributing factor to the successes of solid state theory during the last years have been calculations based on the local density approximation (LDA). It allows to treat a broad range of materials, from semiconductors to simple and transition metals, to molecular solids etc. Fully relativistic calculations are now possible to a precision, which allows understanding e.g. magnetic anisotropies or the occurrence of different crystalline phases from a microscopic point of view. Therefore, solid state theory using this approach will remain a valuable tool for materials science.

However, there are some aspects, which are not satisfactorily addressed by LDA theory. To reproduce the magnitude of band gaps in semiconductors requires the introduction of self-energy corrections. The situation is even more severe for compounds with highly localized valence states, such as oxides. Even though introduction of Coulomb correlation U (abbreviated LDA+U) provides a somewhat better description of such systems, the basic problem of treating the Coulomb correlations comparable to bandwidths remains unsolved. Present day approaches start either from a localized or a band like picture, and introduce other features as corrections, e.g. by perturbative concepts.

As many aspects of electron correlation are very similar in molecules and solids, the question arises as to whether it is not possible to transfer concepts between the two areas in order to make progress in the treatment of electronic correlations. The difficulty encountered is that the ways of treating correlations in small molecules cannot be carried over to solids, in particular for highly localized electrons. Future work should be aimed at overcoming these difficulties, for which ways have been proposed, or to develop novel concepts. Many interesting new ma-

terials show strong electronic correlations. To achieve a satisfactory description of such materials, models have to include the dominant parts of the electron-electron interactions from the start, whereby any theoretical description loses its single particle form. Other important aspects concern the influence of reduced dimensionality on physical properties (mesoscopic phenomena).

5.8.5 . Expected Trends during the Next Years

In U.S., Japan, and Europe there is a broad effort under way to utilize novel phenomena related to electronic structure (in magnetism, superconductivity, etc) for technical applications. This concerns giant magnetoresistance (already used for data storage, but other applications are vigorously pursued), tunnelling magnetoresistance, colossal magnetoresistance (manganites), high T_C materials, and combination of these with each other as well as with existing semiconductor technology. The high potential of new phenomena based on controlled manufacturing of thin films is manifest in the announcement of a joint effort of two major companies (IBM and Infineon) to develop novel magnetic random access memories (MRAM's) within the next 4-5 years.

In Europe, the area of heavy Fermion systems and weak itinerant ferromagnets is studied by very active groups. With regard to high temperature superconductors (high Tc cuprates), giant magnetoresistance (GMR) and colossal magnetoresistance (CMR) in magnetic multilayers and manganites, respectively, the original discoveries were made in Europe. However, activities in the U.S. have grown very strongly in these fields, so that in the future efforts should be made to maintain a competitive position of the European groups.

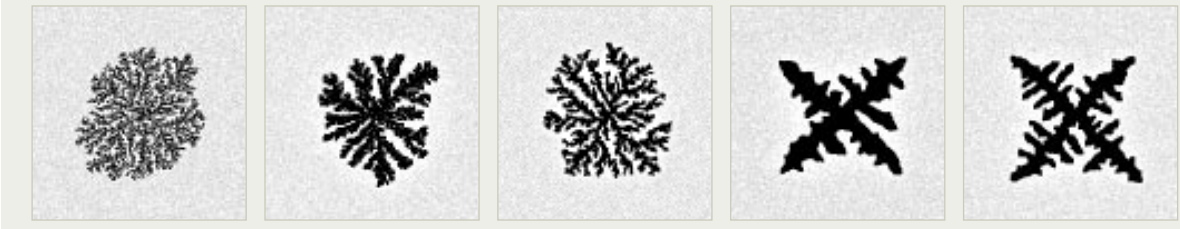
The so-called colossal magnetoresistance materials are attractive for applications because of the large change of the resistance. Basic materials research in this field aims to clarify the underlying physical mechanisms, with the goal of achieving large resistance changes with fields which can be reached in possible device applications.

In many fields future efforts will be directed towards developing phenomena which may reproducible and well understood for narrowly defined, idealized experimental (laboratory) conditions, but need to be extended to wider range of conditions (temperature, pressure, long term stability, etc.) to be useful in applications.

5.8.6. Suggested Measures to be taken by EU

Materials research will be one of the keys to new technologies in the future. To maintain the high level of excellence which has been the achieved in Europe in this area, and to ensure competitiveness in the future, the EU programmes should vigorously support materials research dedicated to understand, develop (improve, optimize) and manipulate (tailor) novel phenomena. This includes among others:
Research on heterostructures: ferro-/non-ferromagnetic, ferromagnetic/semiconductor, oxide-metal interfaces; search for magnetoresistive (GMR, CMR) materials with sharp transitions in small fields at room temperature; spin injection and transport in ferromagnetic/semiconductor structures; synthesis and study of magnetic semiconductors showing ferromagnetic order (GaMnAs and related materials); semimetallic materials; high T_C superconductors and other highly correlated electron systems; micromagnetism, influence of (nano)structuring on properties, superparamagnetic limit, magnetic anisotropy.

Understanding magnetic phenomena on a microscopic level requires advanced analytical techniques, e.g. electron spectroscopies (spin resolution at high-energy resolution, spatial resolution, and time resolution to investigate switching and other dynamical phenomena). Methods for detailed study of spin structures should be developed further, as well as techniques to tailor these for specific needs. Advanced microscopic techniques should



Solidification structure as obtained by computer simulations.

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be developed further to incorporate different contrast mechanisms for the analysis of increasingly complex nanostructured materials. The influence of reduced dimensions on the spin structure both in ferro- and antiferromagnetic materials is important for the basic understanding as well as for applications, and should be studied experimentally as well as theoretically.

In most applications, materials will be employed in the form of thin films. Therefore, surface and interface properties need to be understood and controlled. This requires that studies of bulk properties are complemented by controlled surface and interface preparation and analysis. In addition, special techniques are needed for the analysis of buried interfaces and nanostructured materials.

Dynamic studies of electronic properties, e.g. by using pulsed lasers, are highly desirable. In addition, the time structure inherent to synchrotron radiation offers attractive possibilities for time resolved studies. Also, the use of (soft) X-rays allows differentiating between different components in multilayers or composite materials. Expected pulse widths of the order of 100 fs for projected Free Electron Lasers (e.g. at Hasylab, Hamburg) offer the route to extend these studies to regimes not accessible until now. Use of these unique possibilities should be supported.

In order clarify the similarities and differences in the different classes of strongly correlated materials, research should be extended to more systems showing Fermi liquid instabilities. Microscopic probes such as neutron scattering, probing the short range fluctuations, and muon spin rotation for determining very small magnetic moments should performed, complemented by macroscopic measurements covering extreme conditions, e.g. ultra-low temperatures and high pressures. The study of the influence of substitutions on magnetic and non-magnetic sites in stoichiometric compounds will provide more insight on the (non-) Fermi liquid behaviour of these materials.

Materials science requires the preparation of good materials. Therefore a concerted effort should be envisaged to support the best possible facilities for preparation and characterization of new materials, as well as efforts to prepare 'known' materials with better properties. This includes also preparation and characterisation of micro- and nanostructured systems e.g. by self-organization, e-beam lithography, scanning probe techniques, or other methods.

On the theoretical side, calculations of the electronic structure of diverse materials will be needed in the future to understand and direct experimental studies. Local density functional theory is adequate for many systems of interest, and will remain the prime method to characterise the electronic structure of materials theoretically, at least as a starting point. At the same time, new concepts should be developed to handle highly correlated materials. Many systems of future interest will be non-metallic (oxides, semiconductors), which because of the high degree of electronic correlation are beyond present models, and therefore require refined or even completely novel approaches. To obtain better descriptions of such highly correlated materials, future work should be aimed at incorporating electronic correlations form the start, rather than adding these effects later. Novel schemes to incorporate the effect of self-energy should be developed further.

Despite considerable progress over the last years, it is still not possible to reliably predict the magnetic transition temperatures of ultrathin magnetic films and alloys. Magnetic anisotropy of highly localized compounds and their interfaces is also an issue of increasing importance. These issues should be addressed by theoretical work. The state of art is even less developed for antiferromagnetic and ferrimagnetic systems.

Theoretical models usually deal with idealized situations, which are difficult or impossible to realize experimentally, and much more so for technical applications. Therefore it is desirable to extend theoretical studies to incorporate defects and/or impurities in the bulk and at interfaces, to facilitate comparison to experimental data obtained from non-ideal materials. One of the strengths of European science is the generally close collaboration of experimentalists and theorists. This should also be the practice in the projects funded by the European Commission.

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Conclusions

The number and variety of phenomena displayed by materials are vast, ranging from physical and mechanical phenomena to thermal effects, electronic, optical and magnetic phenomena. Far from equilibrium, complex materials are used nowadays in real applications. We are only beginning to understand the role of the key parameters. Such understanding must increase in the future if we are to design materials with specific properties from the atomic scale upwards. It can be concluded that:

- *Many new phenomena still await to be discovered and to be put on a theoretical basis.*
- *Understanding of dynamical, non-equilibrium aspects of complex systems (from quantum effects to fracture) is a prerequisite.*

The microstructure of a material (crystalline or amorphous; metallic, inorganic, ceramic, organic or biological (living)) controls its properties. There is a strong need to describe changes of the microstructure of materials on the basis of models for the kinetics of material behaviour. Only thus material properties can be optimized. The present state of knowledge does not allow sufficiently accurate modelling of (transformation/reaction) kinetics. In particular:

- *A distinctly improved understanding of nucleation (of new phases) is imperative.*

In forthcoming years undoubtedly the technological importance of thin film systems and nanomaterials will increase still; one could say: the area of minituarization will end only with the emergence of single electron/molecule transistors. Consequently, the interfaces (grain/interphase boundaries) and surfaces may largely dictate the properties of small scale structures. Within this context it has been recognized that there is a lack of basic, fundamental understanding of materials phenomena, that will obstruct further, successful applications of thin films and nanomaterials. In this case certain aspects of both material statics and material dynamics deserve special interest:

- *Data and models for interfacial energies have to be acquired and developed, respectively, in particular for many systems of practical interest.*
- *Interface modelling cannot be achieved on the basis of geometrical/crystallographical concepts alone: transformation constraints, as invariant plane strain, have to be identified and incorporated.*
- *Especially research on interface mobilities has to be promoted. Such work may in particular throw light on the coupling of the thermodynamical driving force to the transformation kinetics.*

An activity of growing importance will be the understanding of the interface of inorganic/metallic material with biological materials. Developments in medical and biological technology necessitate this research.

Small size systems can suffer greatly from lack of stability due to the presence or occurrence of internal stresses. Also against this background, fundamental interest in the consequences of internal stress for material behaviour has grown:

- *An emphasis of research must be on the role of internal (residual) stress in material behaviour.*

Knowledge of materials phenomena on a local (say, atomic) scale by itself does not suffice at all to understand and thus predict material properties of specimens/workpieces on a macroscopic scale:

- *Models for bridging length scales (e.g. for crystalline materials: atom –> domain –> grain –> macroscopic aggregate of grains) have to be developed.*

A well known distinction between materials can be made in view of their application: structural materials, i.e. materials with load bearing capacity, for which the mechanical properties are of cardinal importance, and functional materials, i.e. materials with electrical, magnetic or optical properties of direct use. Microstructural control is the key to their successful application and research in this direction should be encouraged. Thus, development of nanostructured pearlitic steels, i.e. with a very small lamellar distance, could cause superior mechanical properties. Or, control of speed of magnetization reversal in structures of materials of small and smaller becoming dimensions ((laterally structured) thin films and multilayers), used for data storage, requires fundamental understanding of the role of the size parameters.

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Understanding of composites and hybrid materials will be developed to exploit new phenomena for a range of applications from artificial bones to smart materials. Self-repair, environmental sensing and novel electronic, optical and magnetic phenomena are some of the possibilities that could arise from combinations of inorganic/metallic materials and organic/biological materials.

The richness of phenomena exhibited by colloidal systems and solutions needs to be investigated and exploited for the synthesis of materials that are both environmentally benign and superior in performance. Colloidal chemistry is a key technology for fabricating nanostructured, self-replicating and self-assembly materials that will revolutionize the way we manufacture and use materials.

The increasing complexity of materials used in practice (see, for instance, immediately above) requires the availability of models to predict their properties, since it is impossible to enlarge the measured data set of material properties infinitely. Yet, even sophisticated models of this kind require the availability of data sets, for example for boundary, more simple systems, from which successful "extrapolations" can be made. Here one can point at the experimental databases of thermodynamic parameters. The work on these databases is essential for materials science, but its importance is underestimated and certainly not well appreciated. Hence:

- *Data base development, maintenance and linkage should be a coordinated effort and have top priority within the materials science community.*

In the field of materials science in recent years research of applied character has been growing at the cost of research of fundamental character. It is important that basic research on the underlying physical and chemical causes of materials behaviour be invigorated so that we gain sufficient understanding to create the next generation of improved materials. Therefore,

- *Basic, fundamental research on materials phenomena should be promoted.*

A possible European centre of excellence on basic materials science can be crucial for the advancement of fundamental understanding of materials behaviour. Because top level expertise is available at various places in Europe and no existing centre could claim to offer the highest expertise in all areas, it seems appropriate to strive for a virtual centre by linking the top places in Europe. This type of networking can stimulate the progress of understanding enormously by improved interaction between the scientists involved in the centre. Also, the experimental methods in which one institution excels then become available to the whole community in the centre. It would also be advantageous if in such a virtual centre an effort would be made to cross the borders between material classes (e.g. metals and polymers), as the search for unifying concepts for material phenomena should be a focal point of the research activity of the centre.

Finally, Europe should do everything it can to attract more young people for an academic materials science study, in particular a PhD study. The current situation is disastrous. For maintaining, let alone improving, the competitiveness of Europe in basic materials science, this can be as important as the direct funding of this research.

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6. Materials Synthesis and Processing

Introduction

The public at large, confronted with end products based on materials, is largely ignorant of the importance of the necessary processing of the materials on which the product is based. Seldom, also, does it realize the enormous benefits that can result from advances in the processing of materials. Indeed, the costs of materials processing are usually very much larger than the costs of the synthesis of the raw material components. Thus, having knowledge of favourable intrinsic properties of a component (compound) is only the first step in a long development process leading to a successful, practically (i.e. also commercially) important processing route.

Metals were and are still the most important class of materials. Therefore, it is appropriate here to refer to the originally seemingly magical role of the blacksmith in the history of mankind: by using heat and mechanical deformation favourable properties were generated for a workpiece made of a material we (now) call steel. This example serves to illustrate that at least originally the development of knowledge on which a materials processing technology is based was acquired in a phenomenological way, i.e. by chance. Whether the situation has improved may be judged on inspection of the contributions in this chapter. Nowadays many classes of material are manufactured. Although we have striven for a broad coverage, we cannot claim that in the following the processing aspects of all current materials classes of significance have been dealt with extensively. Instead, the focus is on those aspects of materials processing which, with certainty, can be considered to be very relevant currently and which at the same time reveal the general situation and problems associated with materials processing in the European research area. On this basis some general conclusions can be formulated in a reviewing section at the end of this chapter.

◀ Surface of a molten Si sample (optical micrograph obtained using interference contrast, G. Kiessler, MPI für Metallforschung Stuttgart).

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6.1. Thin Film Science

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6.1.1. Introduction

In recent years, thin film science has grown world-wide into a major research area. The importance of coatings and the synthesis of new materials for industry have resulted in a tremendous increase of innovative thin film processing technologies. Currently, this development goes hand-in-hand with the explosion of scientific and technological breakthroughs in microelectronics, optics and nanotechnology [1]. A second major field comprises process technologies for films with thicknesses ranging from one to several microns. These films are essential for a multitude of production areas, such as thermal barrier coatings and wear protections, enhancing service life of tools and to protect materials against thermal and atmospheric influences [2, 3]. Presently, rapidly changing needs for thin film materials and devices are creating new opportunities for the development of new processes, materials and technologies (Fig. 6.1).

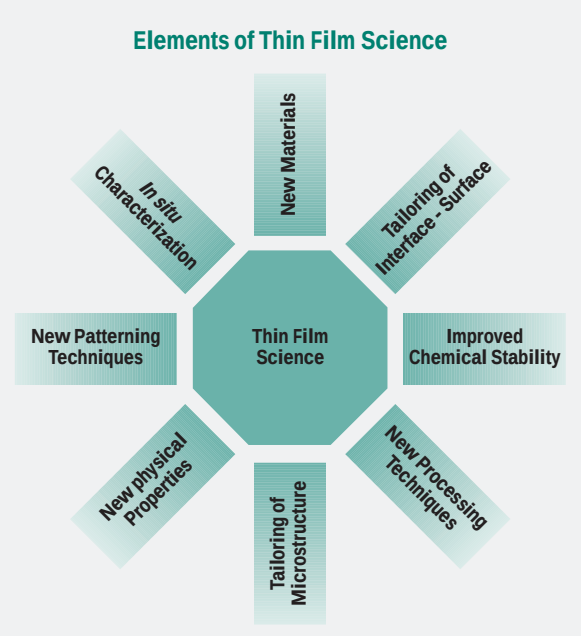

Fig. 6.1. New processing techniques related to thin film materials and devices.

Therefore, basic research activities will be necessary in the future, to increase knowledge, understanding, and to develop predictive capabilities for relating fundamental physical and chemical properties to the microstructure and performance of thin films in various applications. In basic research, special model systems are needed for quantitative investigations of the relevant and fundamental processes in thin film materials science. In particular, these model systems enable the investigation of i.e. nucleation and growth processes, solid state reactions, the thermal and mechanical stability of thin film systems and phase boundaries. Results of combined experimental and theoretical investigations are a prerequisite for the development of new thin film systems and the tailoring of their microstructure and performance.

6.1.2. State of the Art

The major exploitation of thin film science is still in the field of microelectronics. However, there are growing applications in other areas like thin films for optical and magnetic devices, electrochemistry, protective and decorative coatings and catalysis. Most features of these thin film activities are represented by a relatively new research area, called *surface engineering* [2]. *Surface engineering* has been one of the most expanding scientific areas in the last 10 years and includes the design and processing of surface layers and coatings, internal interfaces and their characterization. Surface engineering is directed by the demands of thin film and surface characteristics of materials.

(a) Thin film processing techniques

There exists a huge variety of thin film deposition processes and technologies which originate from purely physical or purely chemical processes. The more important thin film processes are based on liquid phase chemical techniques, gas phase chemical processes, glow discharge processes and evaporation methods [4]. Recently, a considerable number of novel processes that utilize a combination of different processes have been developed. This combination allows a more defined control and tailoring of the microstructure and properties of thin films. Typical processes are e.g. ion beam assisted deposition (IBAD) and plasma enhanced CVD (PECVD). Examples for novel thin film processing techniques, which are still under development, are pulsed laser ablation (PLD) and chemical solution deposition (CSD). Both techniques enable the synthesis of complex thin film materials (complex oxides, carbides, and nitrides).

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Presently, experimental efforts are increasingly supported by computational approaches that address complex growth processes, saving time and money. These approaches enable e.g. the description of the evolution of thin film microstructures as a function of processing parameters.

(b) *In situ* characterization

The thin film process equipment can be categorized into production equipment for device manufacturing, equipment for research and development, and prototype apparatus for fundamental investigations of new or established deposition processes. One reason for the world-wide rapid growth of deposition technology is that equipment manufacturers have successfully met the demands for more sophisticated deposition systems including *in situ* characterization (e.g. reflection high-energy electron diffraction (RHEED), scanning probe microscopy (SPM)) and process monitoring techniques for measuring process parameters and film properties (e. g. ellipsometry, plasma analysis techniques). Novel experimental tools have enabled discoveries of a variety of new phenomena at the nanoscale which have in turn opened unexpected opportunities for the development of thin film systems, and tremendous progress regarding a fundamental understanding of the respective technological processes has been made.

(c) New materials

Thin film systems necessitate direct control of materials on the molecular and atomic scale, including surface modifications, deposition and structuring. Many of these techniques were improved during the last decade, resulting in remarkable advances in the fundamental understanding of the physics and chemistry of thin films, their microstructural evolution and their properties. This progress has led to the development of new materials, expanded applications and new designs of devices and functional thin film systems. One of the most outstanding examples is the successful development of semiconductor devices with novel materials like oxides and nitrides (e.g. GaN). Other typical examples are advances in the synthesis of hard coatings based on borides, carbides and nitrides [3].

6.1.3. Expectations 2000 – 2010

The gap between solving fundamental materials problems and developing new thin film devices for microelectronic and nanotechnological applications is quickly increasing. For example, in many applications the development of thin film systems is accompanied by a variety of materials and processing problems, which require extensive future efforts to be solved. Prominent examples are the adhesion and the thermal and environmental stability of thin film systems. Future developments are critical to overcoming obstacles to miniaturization as feature sizes in devices reach the nanoscale. Basic research in this field will refer to developments of experimental tools necessary to *in situ* characterize and measure thin film structures (e.g. optical and magnetic characterization), and developments of novel techniques for synthesis and design. These techniques may be more reliable, less expensive, or capable of producing films with new or improved properties. Typical examples are chemical solution deposition (CSD), including hydrothermal approaches, biomimetic pathways for assembling inorganic thin films, or device applications of liquid crystalline polymer films [5].

Experiments alone will be insufficient. Theory and modelling are essential for a complete understanding of the fundamental growth and deposition processes. Multiscale modelling of thin film and nanostructuring processes will be an absolute necessity in the next decade in order to utilize the tremendous potential of thin film science and technology. It is expected that time consuming and expensive experiments will be replaced by theory and modelling.

Especially, it is still necessary to develop a fundamental understanding of the decisive growth and deposition processes. It will be important for research institutes to focus on the development of fundamental and novel processes and devices. This will only be realized if a more defined connection of the activities between single research groups and industry can be achieved, based on a fluent exchange of information. Research institutes and companies, which cannot achieve this, will have difficulty competing in future. In this field, Europe must compete directly with the U.S. and Japan. In comparison to Europe, there appears to exist an advantageous research environment in the U.S. and Japan, which supports a more fluent conversion of results from basic research into applications. This could be balanced in Europe by improved networking between industry and research laboratories in the field of basic research.

6.1.4. Expected Needs 2000 – 2010

(a) Initiatives

Emphasis should be placed on future developments of film deposition processes for application in advanced microelectronic device and nanotechnology applications that require the most demanding approaches. Surface engineering is a second important field where similar demands have to be fulfilled. Effective development of thin film

systems can only be realized if the fundamental process steps are well understood. For the future advancement of thin film research and technology, the following endeavors are prerequisite:

- Development of improved and novel thin film process technologies and design methodologies
- Development of new materials
- More fundamental understanding of the relationships between microstructure and properties, and how these can be tailored
- Improvement and automation of *in situ* characterization tools with high spatial resolution and chemical sensitivity
- Strong networking between research laboratories and industry in Europe, and materials research centres in Europe, U.S. and Japan
- Establishment of special competence centres

In the following, some examples are given where new processes and technologies will challenge established procedures:

(b) Thin film model systems

Deposition processes for applications in advanced *microelectronics* and *surface engineering processes* will require the most demanding approaches in the near future. New concepts and design methodologies are needed to create and synthesize new thin film devices and to integrate them into architectures for various operations. Examples are the control of surface processes, the development of computer memory chips, and the production of two- and three-dimensional nanostructures. There will be a rapid increase in the significance of *basic research* projects due to the need of new materials and devices in these fields. Therefore, purposeful future developments and an understanding of the versatility of the basic deposition processes is needed, including microstructural evolution of thin films, e.g. substrate and surface preparation, nucleation and growth. For the realization of thin film systems, it is of future interest to understand the critical role of surfaces and interfaces. We need to know the structure and bonding at heterophase interfaces and grain boundaries, and we have to understand how to produce special interfaces experimentally and how to tailor them for specific properties. Additionally, the thermal, chemical and structural stability of the thin film systems and devices need to be investigated thoroughly to allow for the adaptation of fundamental processes. To initiate all these processes, special model systems have to be synthesized and studied experimentally and theoretically (Fig. 6.2).

Typical examples are:

- metal and ceramic multilayers
- functionally graded thin films
- growth of metastable phase layers
- super hard thin films
- nanocrystalline layers
- superlattice thin films
- composite coatings

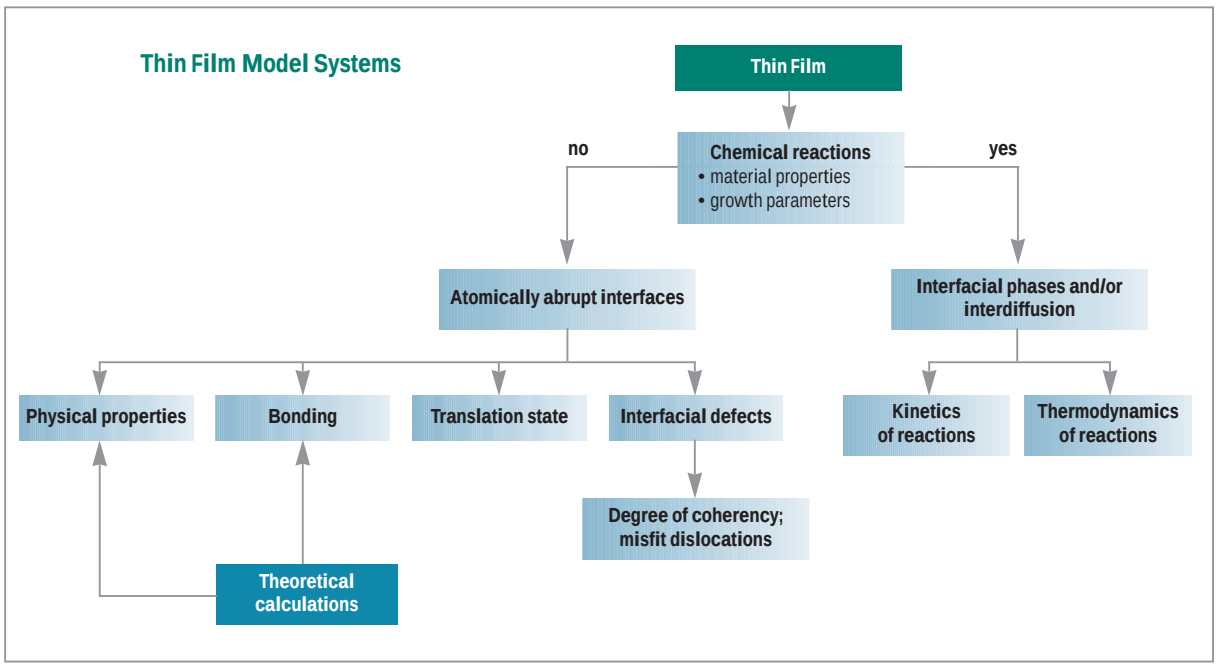

Fig. 6.2. Research areas for thin film systems.

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Significant improvement in both, theory and modelling are necessary to help direct the developments in thin film science and technology. This is one of the most promising attempts for accelerating future developments.

(c) The development of new materials: a combinatorial approach

An accommodation of the equipment to the research and development of new device structures and materials with new properties must be performed continuously. For example, research and development equipment has to offer a high degree of flexibility in the accommodation of a multitude of substrates, in deposition parameters, and in real time monitoring capability. Until recently, these facilities did not facilitate a high product throughput, which made the development of new thin film materials rather tedious. By using a *combinatorial approach*, parallel thin film processing can be realized, and by significantly reducing sample size, time and money can be saved (Fig. 6.3).

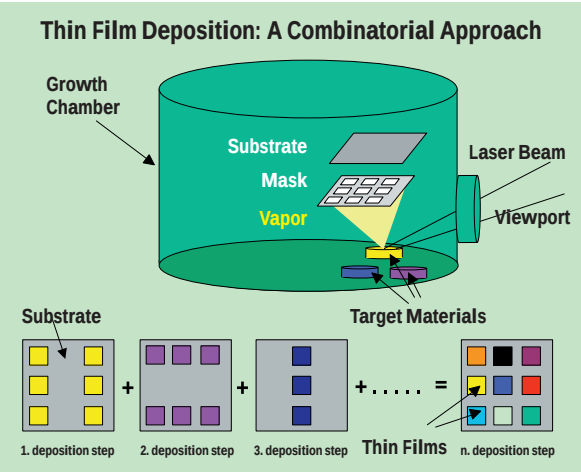

Fig. 6.3. A combinatorial approach for parallel thin film processing.

This requires the development of new and complex deposition systems. For example, this can be realized by using masks with different patterns in front of the substrate. Then, single or/and multi-beam deposition will result in parallel thin film processing. As a result, the substrate will consist of thin film patches with varying chemical composition. However, miniaturization complicates the processing procedures, and thus an improvement in the resolution of typical thin film characterization tools will be of great importance. Full automation of the deposition and characterization routines is required here (e.g. automatic shutter and temperature control, scanning beam RHEED systems). A further advantage of the combinatorial approach is the fast characterization of the deposition process and the system itself. Worldwide, the developments of these processes are still in the initial stages. Presently in Europe, projects of combinatorial chemistry are supported in the field of chemical technologies. These research programmes should be extended to all fields of new technologies, which depend on thin film science, and technology, and it is important to realize these projects in Europe through networks which consist of research centres and industry.

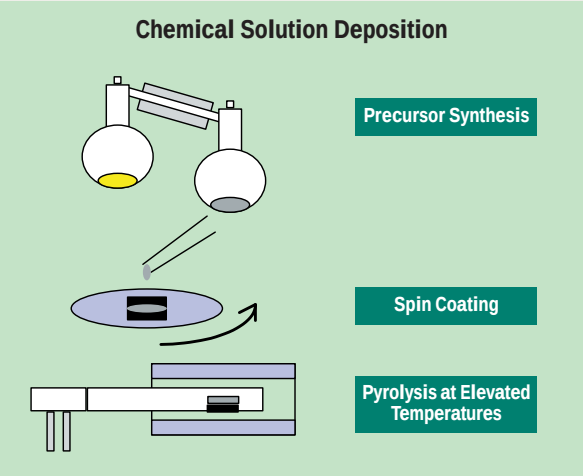

Fig. 6.4. The chemical solution deposition method for the production of epitaxial inorganic thin films.

(d) Thin film systems via chemical solution deposition (CSD)

Conventional CVD and PVD processes are used routinely to synthesize thin film systems. Such process technologies are rather complex and expensive [4]. Depending on the applications, these films have to fulfil special demands and very often, low defect densities are necessary. For most applications, one would prefer films with which have a special texture, low grain boundary density, and smooth surfaces. Epitaxial films fulfil these requirements. Very promising approaches to synthesis inorganic single crystalline thin films are chemical solution deposition method (CSD) (Fig. 6.4) and related processes.

CSD enables the growth of thin films fom solutions, either aqueous or organic [6]. These solutions contain precursor molecules for a variety of elements in the thin film of interest. CSD is inexpensive and enables the synthesis of thin film materials with complex chemical compositions. The main advantage of CSD is the high degree of compositional control, inherent with other solution synthesis routes for multi-element, inorganic materials. Recently, single crystalline carbide and nitride thin films were synthesized via CSD. CSD will become one of the key technologies to synthesize epitaxial oxide, nitride and carbide films for a

variety of different applications, e.g. opto-electronic device applications, hard coatings and dielectric thin films. A further advantage of CSD will be the possibility of direct patterning of thin films via stamping techniques. However, for these purposes, appropriate precursor solutions have to be synthesized in future. One big challenge is the synthesis of precursor materials with well-defined doping levels for thin film applications in electronic devices.

(e) Manpower, interdisciplinary research

Continued progress in thin film research seems to be increasingly dependent upon collaborative efforts among several different disciplines, as well as closer coordination among funding agencies and effective partnerships including research laboratories, universities, and industry. Recently, a variety of different interdisciplinary programmes for nanotechnology and microelectronics were initiated in the U.S., Japan and Europe. However, the topic of thin film science and technology is automatically included in such programmes, although it would be of great benefit to establish individual programmes, which focus on major thin film activities in Europe. Interdisciplinary programmes of *combinatorial materials science and technology of thin films* and *surface engineering* are necessary, to promote the formation of fundamental associations for the improvement and development of new techniques, and of novel materials and their properties.

The university education of researchers working in the thin film area would benefit from an interdisciplinary approach. The materials problems in thin films research are very complex and require interdisciplinary training, that is, a combination of studies including physics, chemistry, engineering, materials science and biology. In comparison to Europe and Japan, the U.S. seems to occupy a leading position in this field. In the future, efforts should be taken to compensate for this deficit in Europe by modifying the education system in such a way that new training directions are included, helping to create a new generation of researchers who work across traditional disciplines. This task may be supported by new centres of excellence in the field of thin film science and technology.

6.1.5. Expenditures

Thin film process techniques and research are strongly related to the basic research activities in nanotechnology. Thus, government expenditures on nanotechnology research are a reliable indicator of the budget for thin film research. The government expenditures for nanotechnology research are presently at similar levels in the U.S., Japan and Western Europe, suggesting that the respective quantities of research activity are comparable. According to a WTEC study in 1997 [1], large companies in Japan and the U.S. contribute to research to a greater extend than do their counterparts in Europe. While large multinational companies are developing nanotechnology research activities worldwide, the transfer of new processes to the market is strongest in the U.S. In Western Europe, a diverse combination of university research, networks and national laboratories with a special emphasis on coatings is active. The largest funding opportunities for nanotechnology are provided by the NSF in the U.S., by MITI in Japan and by BMBF in Germany. Categories such as physical and chemical technologies, materials research, microsystem technologies, electronics and nanotechnologies are supported by BMBF. Common features of these disciplines are projects which are located in the area of thin film research. In the case of nanotechnology, the BMBF has established several centres of competence with emphasis on such topics as opto-electronics, nano-analytics, and ultra-thin films. Ultra-thin films are among the main elements of thin film science that have varied applications in optics, microelectronics and wear protection.

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6.2. Synthesis and Processing of Inorganic Materials

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6.2.1. Introduction

Fundamental to the success of materials science and technology is the availability of high-quality materials exhibiting specific tailor-made properties together with an appropriate shape and microstructure. Let us mention that most of the inorganic materials of current interests have been discovered by chance and it is obvious that there is a conscious effort at present to rationally design inorganic materials based on chemical principles. Although there is a steady progress in solid state chemistry there still exists a serious deficit in the ability to produce materials with desired intrinsic properties by both rational design and synthesis. This remark is also valid for the generation of specific nanostructures, microstructures and shapes, which, eventually, determine the overall performance of a workpiece within a device.

6.2.2. State of the Art

The most important synthetic methods that have been recently developed are molecular templating, synthesis under extreme conditions of pressure and temperature, self-assembly, soft chemistry, electrochemistry, low temperature flux and hydrothermal methods, and the robot-assisted combinatorial synthesis. Most of these new synthetic methods have been essential to allow the isolation of metastable phases with relevant properties. On the other hand, the extraordinary progress in the implementation of sophisticated characterization techniques for the determination of the local chemical composition, texture, microstructure, crystal, electronic, phonon and magnetic structures, has allowed the establishment of precise relationships between crystal chemical parameters, local structure and physical properties. Both, synthesis and composition-structure-property relationships, constitute the feedback for the design of new materials for future needs.

However, despite great advances in probing the structures of solids and measurements of their physical properties, the design and synthesis of inorganic solids possessing desired structures and properties remain a challenge today in both volume and surface dominated materials and in complex systems (Fig. 6.5).

Planning a solid state synthesis rationally includes two basic steps: the prediction of compounds capable of existence, and the design of viable routes for their synthesis. Ideally, one would like to construct a solid compound according to a given requirement profile, and subsequently outline the synthetic route that will produce exactly the required substance. Both these steps are non-trivial because we are not only unable to predict definitely the structure, stability and properties of solid inorganic compounds from first principles, but also we do not know the right method to synthesize the solid even if we have guessed the desired composition. However, an approach towards rational synthesis of inorganic solids could be based on the investigation of the energy landscape of the chemical system using quantum mechanical calculations together with a full understanding of underlying principles of chemical syntheses. Implementing such an approach is still far too difficult, however, and current investigations usually employ a stepping-stone approach by splitting the task into solvable sub-problems using appropriate approximations along the way. First, a global search of the energy landscape constructed from simplified energy functions determines locally ergodic regions, e.g. local minima of the potential energy, which are surrounded by sufficiently high energetic and entropic barriers. These regions correspond to kinetically stable structure candidates, which are then refined on a quantum mechanical level with local optimization methods. In a third step, the properties of these (meta)stable compounds are computed using appropriate algorithms. Finally, a synthesis route for those materials with desired properties is constructed. Besides pointing out the way towards new goals in fundamental and applied chemistry, this study of energy landscapes of chemical systems can assist in the calculation, evaluation and improvement of phase diagrams, by e.g. suggesting possible modifications that exist in synthetically inaccessible regions in the thermodynamic parameter space. These would provide important input data for programme systems like CALPHAD.

Combinatorial chemistry takes its name from a technique in molecular chemistry, where a large number of different molecular building units are placed into solution, allowing the parallel synthesis of essentially all possible combinations of these units. Analogously, many solid state reac-

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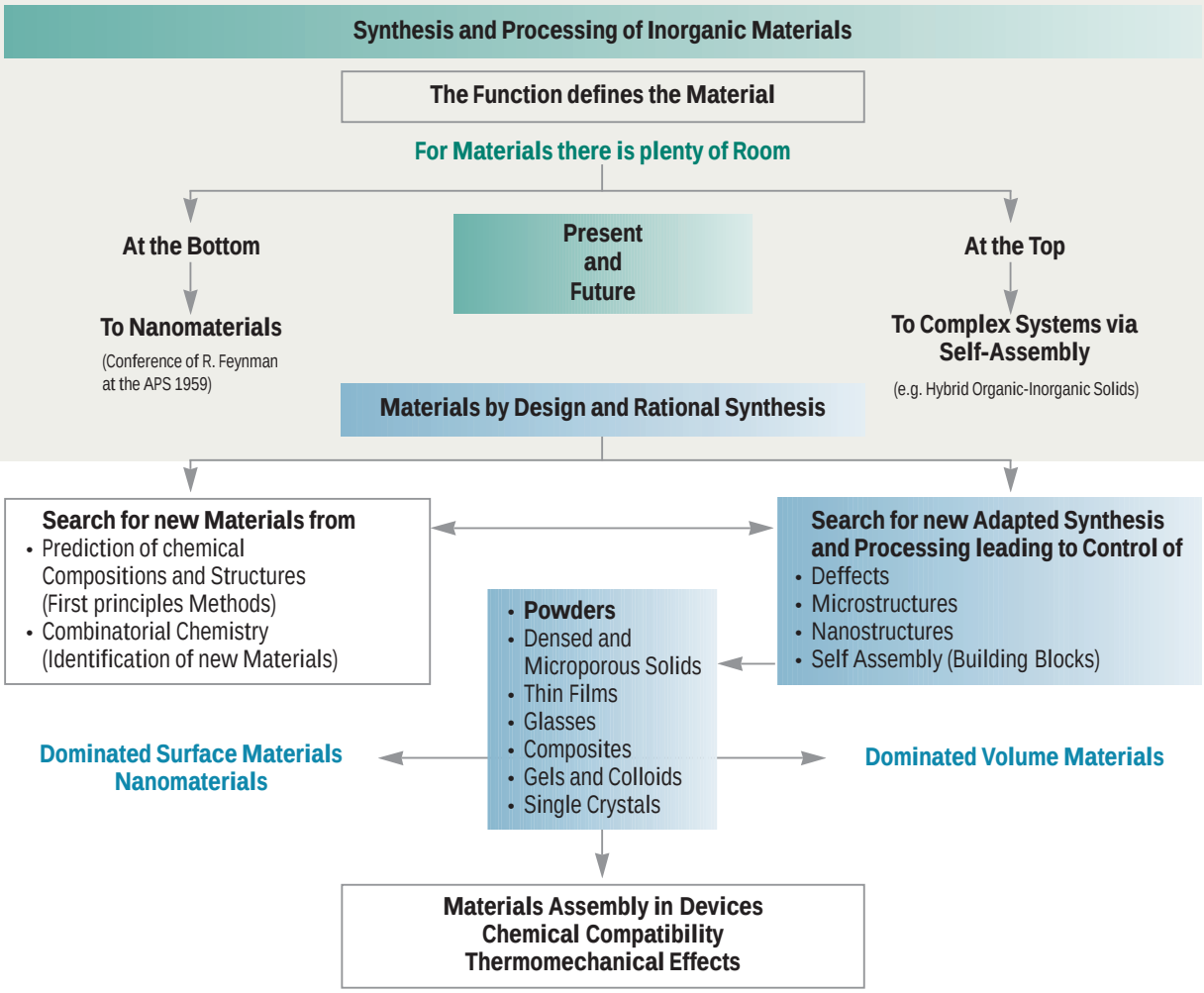

Fig. 6.5. Overview of the synthesis and processing of inorganic materials.

tions are allowed to take place in parallel, spread out over a planar surface, e.g. by thin film deposition combined with multiple masking techniques, or by the solution-phase method employing scanning inkjet techniques. This results in a miniaturization, parallelization and automation of the synthesis. However, since each such a reaction takes place in isolation, for different but fixed compositions, the term « high throughput synthesis » might actually be more appropriate.

The control and the prediction of both textures and microstructures of inorganic materials are crucial for macroscopic properties and industrial applications. When dealing with real systems, non-periodic imperfections play an important role, ranging from defects in single crystals over larger (multi-crystalline) systems containing grain boundaries to macroscopic interfaces and surfaces and finally amorphous compounds, both as film and bulk. These textures and microstructures may occur by accident or design, but the computational resources are usually not sufficient to deal with them from first principles. Thus their description has required the development of various approximations, and semi-empirical and phenomenological models. Usually, the validity of the individual model or approximation is based on the applicability of a separation of time scales, which often translates into a separation on spatial scales. The actual simulations range from quantum mechanical calculations over classical simulations with empirical potentials to finite element methods in continuum mechanics.

Concerning the status of experimental work, currently, mostly physical techniques like e.g. thin- and thick film MBE combined with etching procedures are used when going beyond the crystalline state to achieve specific mesoscopic textures.

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Currently, the EU countries, in particular France and Germany, possess an especially high degree of competence in the area of fundamental solid state chemistry. In contrast, the U.S. and Japan appear to be more efficient in the technology transfer between fundamental science and applied engineering. Let us point out some research fields in which we can compare the competitiveness of Europe vs the U.S. and Japan. In bio-inspired inorganic materials synthesis including organic/inorganic hybrids, U.S. and Europe are very active and Japan has a moderate activity. On the other hand materials by rational design are relatively well-developed in Japanese industry and academic labs by comparison with U.S. which have a moderate and rather decreasing activity. In Europe this type of activity is clearly more important in academic labs than in industry. Combinatorial chemistry for materials discovery (parallel synthesis and screening), is shrinking in U.S. whereas Japanese labs show no or very limited interest for this approach. In Europe this activity is progressing especially in catalytic industry.

In all initiatives taken for developing inorganic materials in different areas (ceramics, nanomaterials, etc.) synthesis and processing are at the heart of the programmes as shown for example by the recent actions launched by U.S. as (i) NSF workshop report devoted to Fundamental Research Needs in Ceramic (April 1999 - NSF Grant # DMR-9714807) (ii) National Nanotechnology initiative: leading to the Next Industrial Revolution (Committee on Technology - National Science and Technology Council - February 2000, Washington D.C.) (iii) Creation of a Centre for Nanoscale Materials at Argonne National Laboratory. It is also noteworthy the big efforts made in Japan on the nanofabrication of materials and nanodevices.

6.2.3. Future Visions and Breakthroughs

As pointed out above, there still exists a serious deficit in the ability to produce (new) materials with desired intrinsic properties and microstructures by rational design. This situation is particularly distressing, since significant progress in science and technology has frequently been triggered by novel materials with outstanding properties as well as by new processing methods. Thus, it is highly desirable to improve efficiency and predictability of solid state chemistry and materials research, not only with respect to generating compounds with new compositions and structures, but also with regard to tailoring their properties. This also holds true for the generation of specific microstructures and shapes, which in the end determine the overall performance of a workpiece within a device.

We note that computational methods can deal with any imaginable chemical system, in principle, but the size and complexity of the systems is limited in the end by the available computational resources and the quality of the algorithms. It is necessary to extend the global optimization stage with simplified energy functions beyond simple ionic systems to larger and more complex compounds. Similarly, on the ab initio level, full local optimizations for all element combinations and comparatively large systems must become routine. Thus, improvements in the efficiency and generality of the first three steps in the approach sketched above are of great importance over the next decade. But the major task for the future is the rational design of synthesis routes, since predicted compounds have to be synthesized in order to verify the calculations and, of course, to make them accessible to applications.

Designing and modelling synthetic routes is much more difficult to achieve than structure prediction. Although synthesis of solids via diffusion processes in close to ideal systems and e.g. chemical vapour deposition can be treated quantitatively, predicting reaction paths on the energy landscape of multicomponent systems still seems to be far out of reach, not to mention steering such reactions through control of external parameters. Thus, even in cases where a new compound and its structure have been predicted, one has to develop individual tailor-made syntheses guided by inspiration and experience.

While being very fast, combinatorial chemistry has difficulties when dealing with a system where no compounds have yet been synthesized, or when the individual syntheses are very sophisticated, as often happens in materials chemistry. Thus, in the future the design of combinatorial equivalents of traditional preparation methods will be crucial for a more general applicability of this method.

Furthermore, one should note, that for materials design the fast automated screening of the reaction products is a very important component of the success of combinatorial chemistry. In order to avoid a bottleneck at this stage, it will be crucial to develop new fast high-throughput screening methods (particular for properties of bulk materials). Finally, we observe that this approach has been restricted to screening thermodynamic space with respect to compositions only, but in the future a systematic parallel exploration of temperature and pressure variation should be implemented.

While there is an obvious element of competition between the rational design described above and the high-throughput synthesis, their particular strengths and weaknesses will most likely result in a rather complementary range of

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applications. Thus, high-throughput will be at its best, if the goal of the optimization of chemical systems can be achieved by tuning compositions and other thermodynamic parameters, while the theoretical approach will be most useful in the exploration of the many « white spots » on the landscape of chemistry.

Interlocking of the various models that are of limited validity on their own will be central for the full theoretical description of mesoscopic textures and microstructures, and the processes that produces them. Experimentally, chemical methods need to be developed that can achieve mesoscopic structures perhaps via self-organized growth using various kinds of templates.

The synthesis and formation of individual nanostructures have many promising opportunities, including dendritic polymers, block copolymers, sol-gel chemistry and controlled crystallization, aerosol nucleation, modified condensation, and nanotube growth. Research into self-assembly, net-shape forming, templating and other manufacturing approaches will allow for a high level of control over the basic building blocks of all materials. An important challenge is to scale up the laboratory processes and develop commercially viable production methods to manufacture stable nanostructures.

6.2.4. Research Needs

1. Synthesis of new materials with promising properties
- Combinatorial chemistry: fast automated screening, new high-throughput syntheses, combinatorial exploration of full thermodynamic space
- Reactions: controlled thermodynamic conditions, including extreme pressures and temperatures, kinetic control in solid state reactions
- Implementation of new synthetic strategies controlling chemical and structural homogeneities at the microscopic scale level and below.

2. Design of microstructure
- Self-organized textures and microstructure
- Hierarchically structured materials
- Local control of size, shape and composition

3. Computational methods
- Global exploration of the configuration space of chemical compounds: applicability to all types of chemical bonding, large and complex systems, rational planning of synthesis routes
- *Ab initio* methods: design of transferable (pseudo-) potentials and basis sets for all elements, full local optimization including cell and atomic coordinates
- Modelling of microstructure: inter-locking of different time and spatial scales, combination of quantum mechanical and classical simulations.

6.3. Synthesis/Processing of Ceramics and Composite Materials

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6.3.1. Introduction

Ceramics are materials roughly defined as non-organic and non-metallic solids, which provide a large range of properties and functions. Most forming methods of organic and metallic parts are generally not suitable for ceramics, due to the brittleness and to the refractarity of ceramic materials. Another essential difference between processing metals and ceramics is that, in the first case, the separation of the industry that produces the material and the industry which fabricates the piece whereas, for ceramics, the same company fabricates the material and the piece.

European laboratories have high competencies in materials (solid state chemistry for instance) but ceramists have to produce pieces using these materials and basic research in ceramic processing appears to be rather poor in Europe. Processing is critical because it generally controls the final properties of the part. With exception of glass, ceramic forming techniques are generally based on powder processing with powder synthesis, forming and sintering. It is then necessary to understand the fundamental mechanisms, which take place during the different steps of the process to obtain reliable and desirable properties of the final parts. Moreover, ceramic processing has also to consider methods that are not based on powder processing including techniques of deposition (chemical and physical) and crystal growth (single-crystal). Then processing research includes thin films and bulk pieces with the development of desirable microstructures and architectures.

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6.3.2. State of the Art

In the last 10 years, advances in ceramic processing have enabled several technological breakthroughs.

The development of new shaping techniques such as rapid prototyping or direct casting allows to design complex architectures adapted to desired improved and/or specific properties. Rapid prototyping techniques (stereolithography, fused deposition, three-dimensional printing, direct ink-jet printing, selective laser sintering...) allow to fabricate net-shape complex ceramic parts, directly from CAD files. Direct casting exploits basic knowledge in colloidal chemistry by using interactions between particles in suspension to transform a well dispersed suspension into a cohesive green body.

The better knowledge of densification mechanisms, the development of sintering models to predict the evolution of microstructure during thermal treatment and the design of microstructure, for instance by using the nucleation and seeding (magnetic ferrite single crystal produced by recrystallization in the solid state, self-reinforced Si_3N_4 and SiC), lead to improved properties.

The synthesis of specific powders and the better control of chemical and of physical characteristics of ceramic powders allow to obtain improved and/or reproducible properties such as mechanical strength of structural ceramics (up to 1000 MPa for zirconia).

In the field of ceramic processing, the efforts have to be directed towards the following domains: 1) synthesis of specific powders, 2) shaping of ceramic components with desirable microstructure and architecture, 3) sintering and microstructure development and 4) surface treatment.

(a) Synthesis of specific powders

The quality of the widely used commercial powders (alumina, zirconia, silicon carbide, silicon nitride, barium titanate) has slowly improved during this last decade. The chemical and physical characteristics are now better controlled but efforts have to be maintained. Then, better properties may be obtained due to more homogeneous microstructures and higher sintered densities. Consecutively, novel processing routes, based on colloidal science, which require constant surface properties, are under development. Moreover, the control of the surface chemistry during the synthesis will lead to improved properties in composite materials.

As far as the particle size is concerned, nanosized particles offer the potential advantage to decrease the sintering temperature and to lead to new properties. One future challenge is the processing of nanoparticles to produce bulk pieces. Nanoparticles should also be included in a matrix, ceramic or not, to fabricate nanocomposites with original properties. This requires the production of nanosized powders, at a commercial level.

Future research needs

1. Synthesis routes to produce specific powders, or homogeneous mixtures of powders, with well controlled chemical (surface) and physical properties (size, shape and surface roughness),
2. Synthesis routes to produce nanosized powders with well-controlled characteristics.

(b) Shaping of ceramic components

The recent efforts, in the domain of ceramic processing, are generally focused on the control of the microstructure but the importance of the architecture is classically underestimated and the conventional approach is limited to the improvement of one specific property. Improved and/or original properties require the design and the achievement of controlled architectures and microstructures. Then, the control of the structure has to be performed over many length scales, ranging from the particle size to the macroscopic dimension of the component. In this context, the creation of new ceramics should be based on a new concept of structure organization at different size-scales by controlling the morphology and the distribution of different building elements (particles, fibres, layers, interfaces, etc.) (Fig. 6.6).

Two ways should be considered to direct the research in shaping of ceramics, first a better understanding of fundamental mechanisms which take place in the different stages of the forming, secondly the development of innovative techniques, for instance, able to produce desirable architectures or miniaturized components. An example concerning the first point is a substantial improvement of the fundamental understanding in the colloid and interfacial science that leads to low-cost techniques such as direct coagulation casting. But, there is a lack of models able to predict the behaviour of a concentrated suspension from knowledge of interparticle forces, particle size distribution and particle shape. Rapid prototyping is an example of the second point. These techniques allow, for instance, to produce functionally graded materials with complex shapes and very small parts with a good dimensional definition (electronic and mechanical components, microelectromechanical systems (MEMS)...). They are also promising for processing fine-scale piezoelectric ceramic/polymer composites allowing for instance to improve the spatial resolution of medical imaging transducers. Nevertheless, these

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new techniques remain under development and an industrial transfer requires an improved knowledge of the different systems used (mixture organic/ceramic) with a better understanding of the role of ceramic/polymer interfaces in processing.

The processing of nanosized powders constitutes one of the greatest challenges for the next years. This requires first, an improved understanding of colloidal behaviour at the nanoscale and secondly, the choice of suitable additives.

A last point to consider is the development of more environmental friendly aqueous systems, even for water sensitive powders (non-oxides, etc.).

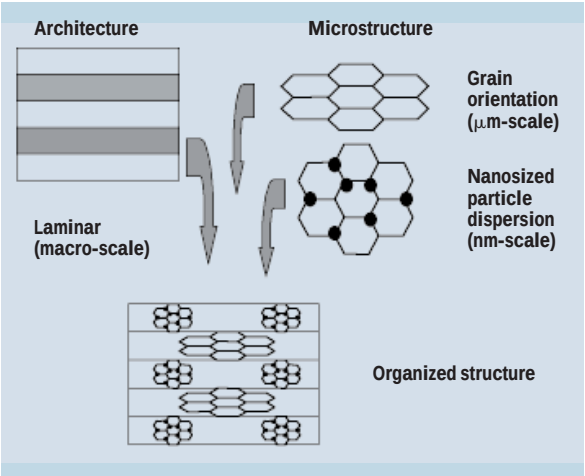

Fig. 6.6. Concept of organized structure (control of different properties).

Future research needs

1. The development of experimental and models to predict the behaviour of a concentrated suspension from knowledge of interparticle forces,
2. The development of innovative shaping techniques to produce desirable architectures and very small parts (mm length scale) with a good dimensional definition,
3. The development of experimental and models to predict the behaviour of nanoparticles concentrated suspensions,
4. The development of aqueous formulations with specific polymers systems.

(c) Sintering and microstructure development

Despite a good qualitative understanding of the microstructure development during sintering leading to a satisfactory control of the sintered microstructure, the rigorous quantitative prediction of solid state sintering behavior is not yet possible for ceramics that are generally complex multiphase systems.

The final objective of the use of nanoparticles is to maintain a nanosized microstructure after sintering in order to obtain improved properties. The understanding of the microstructure development is then critical in this case.

Future research needs

1. The development of models for quantitative prediction of microstructure evolution during sintering,
2. The use of new methods of characterization for quantitative microstructure evolution,
3. The achievement of the basic values of atom diffusivity and surface energy necessary for the model,
4. The development of predictive models of microstructure evolution during sintering of nanoparticles.

(d) Surface treatment

Surface treatment, including deposition of thin ceramic films and thick ceramic coatings, becomes more and more important for electronic devices, thermal and tribological applications. The processing methods for thin films and coatings are specific and largely differ from usual powder processing. The deposition of quality thin films requires the fundamental understanding of nucleation and growth mechanisms of ceramics that influence the microstructure, the surface morphology and stresses. This knowledge could lead to the deposition of microporous thin films which are promising, for instance for dielectric and optical applications.

A future orientation should be likely the deposition of ceramic thin films on polymer substrates that imposes a low temperature process.

Future research needs

1. The fundamental understanding of nucleation and growth mechanisms,
2. The development of low temperature deposition processes,
3. The development of experimental and model of the evolution of stresses during growth of thin films and thick coatings.

6.3.3. Competitiveness of Europe vs. U.S. and Japan in Ceramic Processing

A great part of the American research is focussed on the ceramic processing science for instance for integration of ceramics with other materials (polymers, metals, drugs, etc.). The most important forces in Japan are carried out on new materials with new functions in a wide range of advanced fields (communication, energy, environment, life, etc.) and ceramic processing appears in a second plan.

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At present, the U.S. is likely the main competitor of Europe in the field of processing of ceramic materials, but with research topics more driven by technological applicability than by pure basic scientific curiosity. It is evident that there is a drastic need of fundamental research in ceramic processing in Europe which is poor in comparison to U.S.

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6.4. Synthesis of Polymeric Materials

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6.4.1. Scope of Polymer Synthesis

Synthetic polymers are utilized increasingly in our daily life and manifold industrial applications have contributed to their expansion. Chemical industry devotes a great part of its activity to these polymeric materials. They are employed as substitutes for and /or in combination with metals, glass, ceramics, wood and paper. The worldwide evolution over recent years of the consumption of polymeric materials is given in Fig. 6.7 together with the repartition of the different polymeric materials. The purpose of the present report is to discuss the approaches to design several polymeric materials over a large range of properties. The major part is concerned with a general discussion on these polymerization processes with respect to the nature of the polymerization procedure and its implication on the control of the molar mass and its distribution, the functionality, on the composition for copolymers and on the structural parameters. Selected examples will be presented and discussed more in detail: controlled free radical polymerization, coordination polymerization and the special case of free radical polymerization in emulsion including the recent developments on the polymerization in nano-structured medium. Special attention will be given to the recent breakthroughs in theses polymerization processes. The second part concerns some conclusions and recommendations concerning the future orientations.

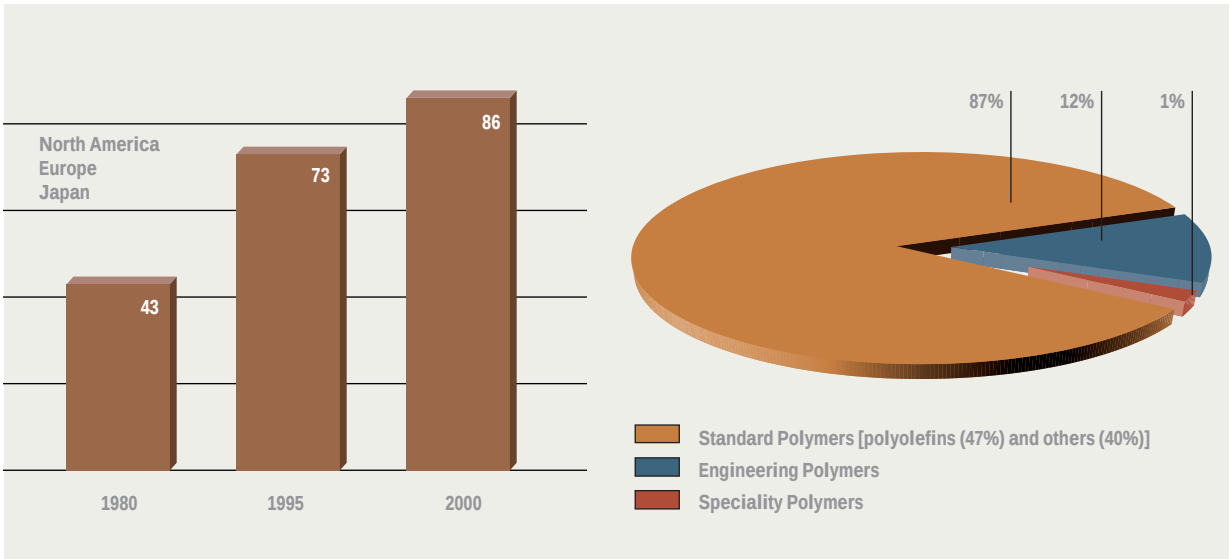

Fig. 6.7. Evolution of plastics consumption (kg/person) in North America, Europe and Japan [1] (a). Worldwide market for plastics in 1996 [1,2] (b).

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6.4.2. State of the Art of Polymer Synthesis Research [1]

(a) Controlled polymerization processes

Anionic polymerization carried out under proper conditions with efficient metal-organic initiators was considered until recently to be the most powerful way to design a large scope of polymers of controlled molar mass, functionality, composition and/or topology. Anionic polymerization has several intrinsic limitations: It requires strict experimental conditions and is only applicable to a limited number of monomers. Therefore the number of materials obtained by anionic polymerization processes is rather restricted. The specific case of the synthesis via anionic stereospecific polymerization of elastomeric materials based on polydienes has to be mentioned. Therefore anionic polymerization remains the method of choice to control the topology of polymers. Two recent breakthroughs in the domain have to be outlined. They concern the good control of the anionic polymerization at high monomer concentrations and the controlled anionic polymerization of meth(acrylic) monomers even at room temperature. These two results obtained in the frame of collaborations with European industrial companies have opened new perspectives for the preparation of well-defined materials. On the contrary, polymerization processes based on *free radical polymerization* are extensively used for the preparation of a large scope of materials in industrial productions. Free radical polymerization is easy to process, can be applied in dilute solution, in suspension or emulsion and even in the bulk. Free radical polymerization is well know to be applicable to a much larger number of monomers. In most cases, that polymerization process leads to high molar masses and does not allow to the control of structural parameters. This is attributed to the short live time of growing sites leading to irreversible termination reactions. Block copolymer synthesis is almost impossible. Many efforts have been devoted recently to obtain a better control of structural parameters in free radical polymerization. New generations of initiators have been introduced in U.S., Japan and also in Europe. These systems called *controlled radical polymerization* [3] based on a reversible termination reaction or a reversible chain transfer reaction controlling the activation deactivation cycles have been subject of increasing interest in the last five years. An equilibrium takes place between the macromolecular radical and a dormant covalent counter part. Pioneering work has been done by Rizzardo [4] and later by Georges [5]. Two systems have emerged: Nitroxide mediated polymerization and Atom Transfer Radical Polymerization (ATRP). They were first applied to homogeneous polymerization processes. Their extension to water represents a major challenge for many polymer chemists. That point will be discussed in the section polymerization processes in nano structured medium. Nitroxide such as those derived from TEMPO (2,2,6,6-tetramethylpiperidinyl) are used for the reversible trapping of growing radicals. At a temperature below 100°C the resulting alkoxyamine is stable whereas at higher temperature the C-O bond undergoes homolitic cleavage thus allowing again the propagation. These systems have been shown to be efficient for controlled polymerization of styrene and substituted styrenes. They are less efficient for acrylic ester monomers. On the contrary phosphonylated nitroxides introduced by Tordo et al (France) in collaboration with Elf-Atochem are well suited for the controlled free radical polymerization of both classes of monomers. Similar work has been performed worldwide by several other groups.

For the ATRP polymerization, copper complexes or ruthenium salts were developed by Matyjaszewski (U.S.) [6] and Sawamoto (Japan) [7] to polymerize vinylic monomers in a controlled way. ATRP is based on the reversible transfer of halogen atoms between dormant alkyl halides and transition metal catalysts by redox chemistry. High molar mass polymers and well-defined block-copolymers could be obtained. The major limitation to the extend the process to industrial applications is due to the presence in the material of inorganic salts or complex ligands.

Reversible Addition Fragmentation Transfer (RAFT) polymerization represents an alternative to the two controlled free radical polymerization processes just described and offers interesting perspectives.

(b) Polymerization and copolymerization of olefins by coordination catalysts

Polymeric materials based on polyethylene (PE) and polypropylene (PP) and their related polymerization processes have attracted increasing interest over the last 50 years. They more and more replace other polymers as they combine low prices with tunable properties and good recycling behaviour. They can be designed for numerous applications such as packaging, textile fibres, automotive parts and even as biomaterials after appropriate modification.

The first decisive step was the discovery by Ziegler-Natta in the 50th of the transition metal catalyzed polymerization of olefins opening new perspectives in the domain of commodity and specialty polymers. Continuous progresses have been made with the aim of improving their efficiency. In the last 20 years new generations of the *heterogene-*

1) A more detailed discussion on the different topics presented in that report is given in the following reference:
Materials Science and Technology, A Comprehensive Treatment, Volume Synthesis of Polymers, Ed. A.D. Schlüter, Wiley-VCH Weinheim-New-York (1999)

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ous Ziegler-Natta based catalysts have been introduced in Europe, Japan and in the US. Important cost reductions could be obtained with the 3rd and 4th generation of Ziegler-Natta catalysts based on titanium trichloride/magnesium chloride in the presence two Lewis bases. These catalysts are highly stereospecific and very active.

In the 80's the introduction by Kaminsky [2](Germany) of the *homogeneous* catalysis based on metallocenes and activated by methylaluminoxane was expected to revolution the domain of organometallic chemistry, polymer synthesis and processing. The driving force for the use of these catalysts is the existence of single-site feature enabling the precise control of molecular parameters: narrow molar mass distribution, chemical composition and microstructure [8,9]. New tailor-made polymers could be obtained and some products based on metallocene catalysts are now on the marked including some types of isotactic polypropylenes.

The discovery in industrial companies in Europe and later in the U.S. of the late transition metal complexes less oxophilic compounds and therefore less sensitive to polar media. These catalysts have generated considerable interest for the polymerization and copolymerization of olefins with polar and especially acrylic monomers [10,11]. In the 1995s Brookhart and co-workers have developed a new generation of palladium and nickel (late transition metals) catalysts aimed either at the polymerization of olefins or at the copolymerization of olefins with some acrylates. The incorporation of functional groups into hydrocarbon polymers constitutes an interesting approach for modifying the chemical and physical properties of these polymers, such as permeability, compatibility, dyeability, adhesion, solid state morphology, and rheology. The same generation of catalysts has been shown to provide access to poly(olefins) of controlled topology.

(c) Polymerization in nanostructured media[2]

Free radical polymerization in colloidal dispersions such as emulsions has been increasingly used over more than 50 years to design in industrial processes numerous intermediates for paints adhesives polishes and coating materials. That polymerization process has been subject of constant interest and even, if some problems are still open, particles of controlled size and functionality are now easily accessible. In the 80s the concept of microemulsion polymerization has been introduced. That polymerization in nano-structured media (micelles, microemulsions) based on classical free radical polymerization represents a important progress in controlled synthesis of functional polymers carrying hydrophobic and or ionic sites. The specific features of the processes – small size of the droplets and large overall and large interfacial aria – result in a unique microenvironment which can be taken advantage of the product to produce novel materials with widely different properties designed for a large scope of applications [12]. The polymerization in aqueous emulsion or suspension to design materials directly in water for various applications such as painting/coating. Increasing interest has been devoted to such (co-polymerization) reactions in water who constitutes an ideal medium for at least two reasons: environment and safety. Presently such arguments are very important in most countries. Beside the classical free radical polymerization, it has been shown that ATRP is also applicable in emulsion. In addition it has to be mentioned that amphiphilic block copolymers were designed by ATRP or nitroxide mediated polymerization as stabilizers in the free radical polymerization emulsion of styrene.

These reactions are yet limited to polymers where no tacticity control is required. Only recently work has been done to develop efficient catalytic systems for the polymerization of olefins in water. Pioneer work on coordination polymerization in water has been done in the group of Lyon in collaboration with Elf Atochem. Emulsion polymerization of ethylene polymerization using bimolecular P,O-chelated ligands based on nickel yielded in aqueous dispersed medium latexes of HDPE. Similar work has been done in Germany to prepare with palladium catalysts branched poly(ethylenes).

6.4.3. Future Visions and Expected Breakthroughs

In the present report the most important polymerization processes have been presented and their contribution to the preparation of materials covering a large range of properties discussed.

The preparation of well-defined linear homo or block copolymers including functional polymers via *controlled free radical polymerization* is now well possible for an extended number of monomers and therefore provides access to various materials. The stereospecific controlled free radical polymerization remains a major challenge and work should be done along that line. The combination of controlled free radical polymerization procedures with a *polymerization in emulsion* (or in nano-structured medium) has been shown to access materials of controlled structural parameters directly in water. That domain should be examined thoroughly in the near future.

2) A detailed overview of the present situation in the domain of polymerization in dispersed medium is given in the following reference : Macromol. Symp. 150, 2000.

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The possibility to design polyolefins with controlled branching or containing controlled amounts of polar monomers by low pressure polymerization processes represents also attractive perspectives for the low cost industrial preparation of materials. The search for new families of non metallocene catalysts with enlarged possibilities should be supported.

The possibility to polymerize olefins in water has been demonstrated. Further work in that direction should be strongly supported in Europe. The heterogeneization of metallocenes catalysts represents also an important challenge.

Many other possibilities or polymerization conditions /reactions exist or are under investigation for the preparation of polymeric materials. Among these, the chemistry in the molten state has to be mentioned, this concerns the chemical modification of polymers and their synthesis starting from monomers. Along the same line the polymerization in supercritical carbon dioxide constitutes a great deal. The increasing contribution of various polymerization processes to the synthesis of polymeric biomaterials of controlled characteristics has to be highlighted.

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6.5. Metal-Matrix Composites: Challenges and Opportunities

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6.5.1. Scope and Definitions

A metal matrix composite (MMC) combines into a single material a metallic base with a reinforcing constituent, which is usually non-metallic and is commonly a ceramic. By definition, MMCs are produced by means of processes other than conventional metal alloying. Like their polymer matrix counterparts, these composites are often produced by combining two pre-existing constituents (e.g. a metal and a ceramic fibre). Processes commonly used include powder metallurgy, diffusion bonding, liquid phase sintering, squeeze-infiltration and stir-casting. Alternatively, the typically high reactivity of metals at processing temperatures can be exploited to form the reinforcement and/or the matrix *in situ*, i.e. by chemical reaction within a precursor of the composite.

There are several reasons why MMCs have generated considerable interest within the materials community for nearly 30 years:

1. The "composite" approach to metallurgical processing is the only pathway for the production of entire classes of metallic materials. Only in this way can aluminium, copper, or magnesium be combined with significant volume fractions of carbide, oxide or nitride phases because, unlike iron, the solubility of carbon, nitrogen or oxygen in the molten metal is (with the exception of O in Cu) far too low.

2. The approach facilitates significant alterations in the physical properties of metallic materials. Composites offer scope for exceeding the specific elastic modulus value of about 26 J kg^{-1}, which is exhibited by all the main engineering metals. Composites also offer the only pathway for producing materials with tailored physical property combinations: an example is that of low thermal expansivity combined with high thermal conductivity, a combination of importance for electronic packaging.

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3. MMCs offer significant improvements over their polymer matrix counterparts with regard to several properties, including tolerance of high temperature, transverse strength, chemical inertness, hardness and wear resistance, while significantly outperforming ceramic matrix composites in terms of toughness and ductility.

4. Exceptional properties can be obtained in some cases. An example is that of 3M's Nextel-reinforced aluminium composites, which exhibit along the fibre direction a tensile strength of 1.5 GPa, a compressive strength of 3 GPa and a transverse strength above 200 MPa, in a material of density only slightly above 3 g cm^{-3}.

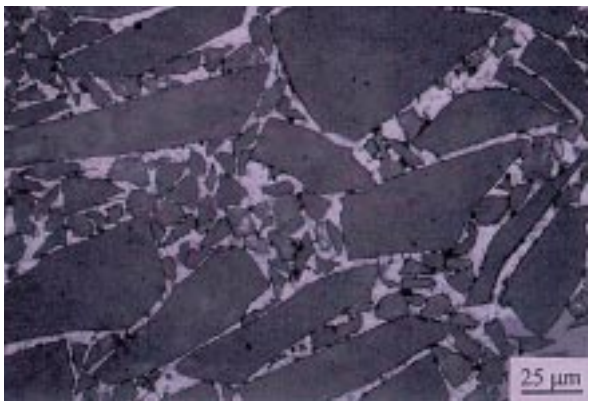

Fig. 6.8. Duplex particle size distribution in a commercially available 70vol% (PRIMEX) SiC particle reinforced aluminium MMC for electronic substrate application.

MMCs come in several distinct classes, generally defined with reference to the shape of their reinforcement:

Particle-Reinforced metals (PRMs) contain approximately equiaxed reinforcements, with an aspect less than about 5. These are generally ceramic (SiC, Al_2O_3, etc.). PRMs commonly contain below 25vol.% ceramic reinforcement when used for structural applications, but can have as much as 80vol% ceramic when used for electronic packaging (Fig. 6.8). In general, PRMs are at least approximately isotropic. They are produced using both solid state (powder metallurgy) and liquid metal techniques (stir casting, infiltration). Their mechanical properties, while often inferior to those of fibre-reinforced metals, are more or less isotropic and often represent, at moderate cost, significant improvements over those of corresponding unreinforced metals.

Short Fibre- and Whisker-Reinforced metals. These contain reinforcements with an aspect ratio of greater than 5, but are not continuous. These composites are commonly produced by squeeze infiltration. They often form part of a locally reinforced component, generally produced to net or near-net shape. Their use in automotive engines is now well established.

Continuous Fibre-Reinforced Metals contain continuous fibres (of alumina, SiC, carbon, etc.) with a diameter below about 20 µm. The fibres can either be parallel, or pre-woven before production of the composite; this is generally achieved by squeeze infiltration.

Monofilament-Reinforced metals contain fibres that are relatively large in diameter (typically around 100 µm), available as individual elements. Due to their thickness, the bending flexibility of monofilaments is low, which limits the range of shapes that can be produced. Monofilament-reinforced metals can be produced by solid state processes requiring diffusion bonding: they are commonly based on titanium alloy matrices, which are well-suited to such techniques.

Interpenetrating phase composites are ones in which the metal is reinforced with a three-dimensionally percolating phase, for example ceramic foam.

Liquid phase sintered metallic materials, include the cemented carbides, in which carbide particles are bonded together by a metal such as cobalt, and the tungsten heavy alloys.

6.5.2. State of the Art

MMCs have been extensively studied. SiC monofilament-reinforced titanium has been the subject of many investigations, as have aluminium alloys containing up to 25 vol% SiC and Al_2O_3 particles. These materials have been produced by industry (including Alcan, Textron, Alcoa, AMC, BP, and 3M) in relatively large quantities, such that they have been made available for testing at research laboratories and universities. Their novelty, and their interesting mechanical behaviour (at both micro- and macroscopic levels), have led to many publications, exploring many features of their microstructure, deformation, and fracture behaviour. Many mechanisms responsible for their mechanical characteristics are now well understood, including the roles of damage development, internal stresses, reinforcement clustering, interfacial bond strength and the effects of the presence of the reinforcement on aging of the matrix. However, much work remains to be done before required property combinations can be systematically achieved via microstructural design.

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The processing of MMCs has also generated much interest. Many publications have appeared over the past decades on this subject. Commonly, such studies have presented novel composite materials or processes, without advancing the underlying science concerning the transport phenomena involved or their relationship with microstructural features of the product. For example the rate of solid state consolidation of a mixture of two different powders is not yet predictable, nor is the rate of liquid phase sintering of metal bonded carbides.

With regard to industrial applications, MMCs now have a proven track record as successful "high-tech" materials in a range of applications, bringing significant benefits (in terms of energy savings, or component lifetime) and having documented engineering viability. These often relate to niche applications, where achievable property combinations (e.g. high specific stiffness and weldability; high thermal conductivity and low thermal expansion, or high wear resistance and low weight and high thermal conductivity) are attractive for the component concerned. Many such niches, ranging from diesel engine pistons to automotive engine cylinder liners, are of considerable industrial significance. Barriers to their wider exploitation include price (which is, of course, inter-related with global and specific usage levels), shortage of property data and design guidelines and (perceived) limitations to their ductility and toughness.

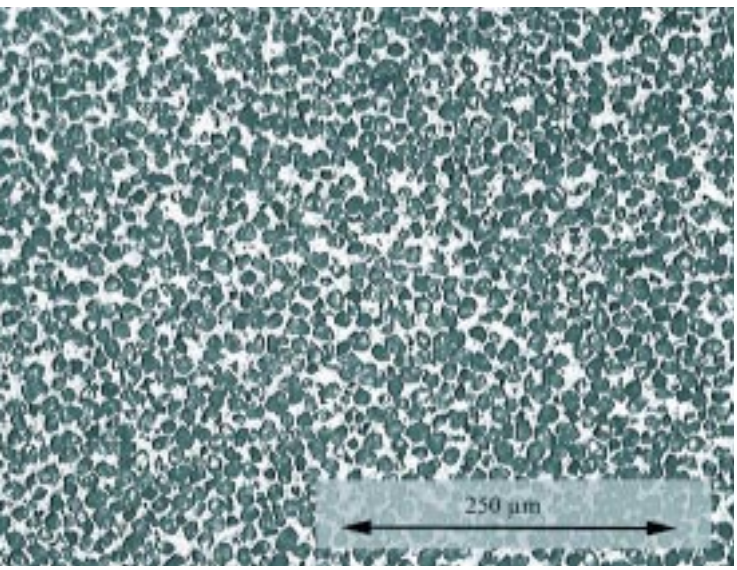

Fig. 6.9. Optical micrograph of a pressure-infiltrated composite combining pure aluminium with high-performance alumina particles: this material, despite its high ceramic content, displays a tensile elongation of 4.5% and a toughness on the order of 25 MPa√m.

6.5.3. Challenges and Opportunities: Priorities in European Research

Several challenges must be overcome in order to enhance the engineering usage of MMCs. Research efforts required to overcome these challenges span the spectrum from basic, fundamentals-oriented research, to more applied engineering projects.

1. There is a need to advance our understanding of processing fundamentals, particularly concerning established processes such as squeeze infiltration, liquid phase sintering, and powder metallurgy. Progress in this area is required, both to drive innovation and to enable quantitative process simulation, optimization, and control. In particular, progress in this area is critical for controlling internal defects – an important goal with these materials, given that they are more brittle than unreinforced metals.

2. Property improvements must be sought, particularly in ductility and toughness. Systematic investigations are required of the fundamental links between microstructure and properties. Much work to date has focused on only a few commercial or near-commercial materials, which have been characterized in detail, but do not provide full insight into basic microstructure-property relations, such as the link between particle size or spatial distribution and mechanical properties.

3. There is clearly scope for improvements in the properties of reinforcements. Substantial advances in fibres for MMCs have been achieved at the 3M company: in terms of strength, for example, the performance of alumina fibre-reinforced aluminium has *doubled* over the past decade. Recent work has also shown that significant differences exist between ceramic particles that can be used as reinforcements for aluminium (Fig. 6.9). Research on the economical production of high strength, low-cost, ceramics for the reinforcement of metals would be very timely.

4. An important issue concerns secondary processing. Operations such as welding and machining, and also the definition of recycling strategies, are challenging when applied to MMCs. Research in this area is critical for certain applications and for the life-cycle engineering of these materials.

5. Much work to date has focused on aluminium matrix composites, but copper, magnesium, and iron-based matrix composites do offer promise in specific applications. These include electronic applications for copper-

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matrix composites, and chemical processing environments for steel matrix composites. These systems deserve exploration, again with emphasis on fundamentals, rather than the development of this or that specific composite.

These windows of opportunity in research are ones which, in large part, call for partnerships between different laboratories and researchers. For instance, a capability for controlled processing of these materials is needed for the generation of samples and microstructures that can be used in the exploration of microstructure-property relations. Unlike unreinforced alloys, in which the microstructure can be varied using conventional and well-established deformation and heat-treatment processes, the processing of MMCs requires specialized equipment and know-how. The establishment of a European centre of excellence in MMC research, able to cover the entire spectrum from processing to performance, and providing a hub for such a coordinated effort, would be highly opportune.

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6.6. Ceramic Matrix Composites

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6.6.1. Introduction

Ceramic matrix composites (CMCs) have been developed to overcome the intrinsic brittleness and lack of reliability of monolithic ceramics, with a view to introduce ceramics in structural parts used in severe environments, such as rocket and jet engines, gas turbines for power plants, heat shields for space vehicles, fusion reactor first wall, aircraft brakes, heat treatment furnaces, etc. It is generally admitted that the use of CMCs in advanced engines will allow an increase of the temperature at which the engine can be operated and eventually the elimination of the cooling fluids, both resulting in an increase of yield. Further, the use of light CMCs in place of heavy superalloys is expected to yield significant weight saving. Although CMCs are promising thermostructural materials, their applications are still limited by the lack of suitable reinforcements, processing difficulties, sound material data bases, lifetime and cost.

6.6.2. Ceramic Matrix Composite Spectrum

A given ceramic matrix can be reinforced with either *discontinuous* reinforcements, such as particles, whiskers or chopped fibres, or with *continuous* fibres. In the first case, the enhancement of the mechanical properties, in terms of failure strength and toughness, is relatively limited but it can be significant enough for specific applications, a well known example being the use of ceramics reinforced with short fibres in the field of the cutting tools (SiC_w/Si_3N_4 composites). Among the discontinuous reinforcements, whiskers are by far the most attractive in terms of mechanical properties. Unfortunately, their use raises important health problems both during processing and in service. Conversely, continuous reinforcements, such as fibre yarns, are much more efficient, from a mechanical standpoint, but they are more expensive and more difficult to use in a ceramic matrix in terms of material design and processing.

There is a wide spectrum of CMCs depending on the chemical composition of the matrix and reinforcement. *Non-oxide* CMCs are by far those which have been the most studied. Such a choice could appear surprising since the atmosphere in service is often oxidizing. That choice could be explained as follows. The most performant fibres, in terms of stiffness, failure strength, refractoriness and density are non-oxide fibres, i.e. carbon and silicon carbide fibres. Further, carbon fibres are extensively used in volume production of polymer-matrix composites. As a result, they are much cheaper than all the other fibres (glass fibres excepted). Second, in order to avoid compatibility

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problems, which are crucial at high temperatures, non-oxide fibres are preferably embedded in non-oxide matrices. Hence, the first non-oxide CMCs have been *carbon/carbon* (C/C) composites. They have been initially designed and produced for use in rocket engines and re-entry heat shields, i.e. under extremely severe service conditions but short lifetimes. In a second step, *C/SiC* and *SiC/SiC* composites were developed in order to increase the oxidation resistance of the materials and hence their lifetimes in oxidizing atmospheres. Silicon nitride was also used as matrix although it is less stable at high temperatures than silicon carbide.

Oxide-CMCs would obviously be the best choice, from a thermodynamic standpoint, for long term applications in oxidizing atmospheres. Unfortunately, oxide fibres, although they are refractory, tend to undergo grain growth at high temperatures, (which results in a fibre strength degradation) and exhibit a poor creep resistance. Further, they display much higher densities than say carbon fibres (4 g/cm^3 for alumina versus 2 for carbon). Attempts have been made to improve the high temperature properties of oxide fibres with limited success. Despite these disadvantages, Al_2O_3/Al_2O_3 and derived CMCs have been, and are still, extensively studied.

6.6.3. State of the Art in CMC Processing

CMCs can be produced according to either *gas phase* routes or *liquid phase* routes, each of them having advantages and drawbacks.

In *gas phase routes*, i.e. the so-called chemical vapor infiltration (CVI) processes, the reinforcements (usually as a multidirectional preform) is densified by the matrix deposited from a gaseous precursor, e.g. an hydrocarbon for carbon or a mixture of methyltrichlorosilane and hydrogen for silicon carbide. It is now well established that a fibre coating, referred to as the interphase, has to be deposited on the fibre prior to the infiltration of the matrix in order to control the fibre-matrix (FM) bonding and the mechanical behavior of the composite. Pyrocarbon (PyC), boron nitride or (PyC-SiC)n and (BN-PyC)n multilayers, with an overall thickness ranging from about 0.1 µm to about 1 µm, displaying a layered crystal structure (PyC, BN) or a layered microstructure (multilayers), are the most common interphase materials in non-oxide CMCs. The main role of the interphase is to deflect the microcracks which form in the matrix under loading and hence to protect the fibre form notch effect (mechanical fuse function).

There are several versions of the CVI-process. The most commonly studied and used version is isothermal/isobaric CVI (or I-CVI). It is a relatively slow process since mass transfer in the preform is mainly by diffusion and it yields some residual porosity and density gradient. Conversely, I-CVI is a clean and flexible process (it can be used to densify simultaneously a large number of preforms, eventually of different shapes). For these reasons, it is the preferred process at the plant level. It is well suited to the fabrication of relatively thin parts.

In order to increase the densification rate and hence to reduce the processing times, temperature or/and pressure gradients can be applied to the preform. In temperature gradient CVI (TG-CVI), or forced CVI (F-CVI), the processing time can be reduced by one order of magnitude with respect to I-CVI. A similar processing time lowering has also been reported for the film-boiling (or calefaction) process, in which the heated fibre preform is directly immersed in a liquid matrix precursor.

Finally, pressure pulsed-CVI (P-CVI) has been recently presented as a way to engineer, at the micrometre (or even nanometre) scale, either the interphase or the matrix. Based on this technique, multilayered *self-healing* interphases and matrices (combining crack arrester layers and glass former layers) have been designed and produced, through a proper selection of chemical composition of the layers. An example of such highly tailored composites is shown in Fig. 6.10.

Fig. 6.10. Example of multilayered self-healing matrix ceramic matrix composite produced by P-CVI. The matrix comprises crack arrester layers and glass-forming layers.

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In the *liquid phase routes*, the fibres first coated with an interphase (e.g. by I-CVI) are embedded in a liquid precursor of the matrix. In the *reactive melt infiltration* (RMI) processes, a fibre preform is impregnated by capillary forces with a liquid which reacts either with a solid phase used to consolidate the fibre preform (SiC-Si matrices formed through liquid silicon infiltration of a carbon-consolidated preform) or with the atmosphere (Al_2O_3-Al matrices formed through liquid aluminium infiltration and chemical reaction with an oxidizing atmosphere). Among other advantages, the RMI-processes are fast and can be applied to thick preforms. They also yield materials of low residual porosities and high thermal conductivities.

In the *polymer impregnation and pyrolysis* (PIP) processes, the fibres are embedded in a polymeric precursor of the matrix, such as a thermosetting resin or a pitch for carbon or a polycarbosilane for SiC, and the green composite is then pyrolyzed. Such processes are relatively flexible since the composition of the precursor can be tailored. Conversely, a shrinking of the matrix occurs during the pyrolysis step owing to the evolution of gaseous species. As a result, several PIP-sequences have to be applied in order to achieve a low enough residual porosity, which is time and labour consuming. Shrinkage can be limited by loading the liquid precursor with suitable fine powder, i.e. by using a slurry. Finally, the residual porosity can also significantly be reduced through a hot pressing step, an alternative that supposes that the matrix displays enough plasticity not to damage the fibres. This liquid impregnation/hot pressing technique is well suited to the fabrication of glass-ceramic matrix composites.

6.6.4. Expected Breakthroughs and Future Visions

The future of CMCs is directly depending on progress that would be achieved in the availability of higher performance constituents (fibres, interphases and tailored matrices) as well as in processing cost reduction.

As far as the *reinforcements* are concerned, two main breakthroughs are expected : (i) the availability of a *low cost* non-oxide fibre that could be used up to about 1500°C and (ii) the development of a refractory oxide fibre resistant to grain growth and creep. Oxygen-free quasi-stoichiometric SiC fibres display much better high temperature properties than their Si-C-O counterparts fabricated from polycarbosilane according to the Yajima's route. However, they are too costly (with respect to carbon fibres and CMC volume production) and their failure strain is too low. Amorphous Si-B-C-N fibres, presented as creep resistant at high temperature, are still at a development stage. Although alumina-based binary oxide fibres, e.g. mullite/alumina or alumina/YAG fibres, represent a significant progress in terms of creep resistance with respect to pure α-alumina fibres, further improvement is still necessary to match the high temperature properties of non-oxide fibres. Finally, nanotubes, with their outstanding mechanical properties, may raise problems similar to those previously encountered with whiskers.

The spectrum of suitable *interphase materials* that could be used in a realistic manner in CMCs remains extremely narrow. In non-oxide CMCs, there is presently no alternative to the carbon-based interphases. Boron nitride is obviously the only potential candidate. However, its sensitivity to moisture when poorly crystallized and its low bonding to SiC-based fibres are subjects of concern. Solving these two problems will be an interesting breakthrough. The search for new interphase materials, displaying a better oxidation resistance than carbon and boron nitride and which could be easily deposited *in situ* in multidirecitonal fibre preforms, should be strongly encouraged.

The recent discovery of the *self-healing multilayered matrices* (Fig. 6.10) has been an important breakthrough since it permits the use of non-oxide CMCs in oxidizing atmospheres. The concept should obviously be further developed in terms of material selection.

Finally, the processing cost of CMCs should be reduced (although the main contribution to the total cost of a given part is presently, e.g. in a SiC/SiC composite, that of the reinforcement, as previously mentioned). Gas phase route processes with a significant reduction of the overall densification time, liquid phase route processes with a limited number of PIP-sequences (through the use of appropriate precursors), both being compatible with CMC volume production, would obviously be significant breakthroughs.

6.6.5. Future Directions of Research

The interest of CMCs as thermostructural ceramics is now well established but their volume production at the plant level is still a challenge, which requires an important effort of research at the level of the European Union. Possible directions of research are :

- Development of *low cost ceramic fibres* (both non-oxide and oxide fibers) that could be used up to about 1500°C (the EU has presently no long term action that could be compared to what is done in Japan and U.S.).

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- Development of *one or two* CMC(s), e.g. a SiC-based and an alumina-based composites, including that of an interphase material and a low cost processing technique, guided by one or two potential application(s).
- Development of sound *data bases* on CMCs and their constituents (including that of suitable standard tests and modelling).
- Development of the *durability* of CMCs, including that of suitable internal and external oxidation protection (for non-oxide CMCs), lifetime prediction, residual mechanical and thermal properties characterization and modelling.

6.7. Polymeric Composite Materials

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6.7.1. Introduction

Principal advantage of composite materials resides in the possibility of combining physical properties of the constituents to obtain new structural or functional properties. Composite materials appeared very early in human technology, the "structural" properties of straw were combined with a clay matrix to produce the first construction material and, more recently, steel reinforcement opened the way to the ferroconcrete that is the last century dominant material in civil engineering. As a matter of fact, the modern development of polymeric materials and high modulus fibres (carbon, aramidic) introduced a new generation of composites. The most relevant benefit has been the possibility of energetically convenient manufacturing associated with the low weight features. Due to the possibility of designing properties, composite materials have been widely used, in the recent past, when stiffness/weight, strength/weight, ability to tailor structural performances and thermal expansion, corrosion resistance and fatigue resistance are required. Polymeric composites were mainly developed for aerospace applications where the reduction of the weight was the principal objective, irrespective of the cost. The scientific efforts in this field were therefore focused to the comprehension and optimization of the structural performances of these materials. Structural composite materials have been also used in other fields such as automotive, naval transportation and civil engineering but the high cost still limits their applications. A continuous task has been making composite components economically attractive. The effort to produce economic attractive composite components has resulted in several innovative manufacturing techniques currently being used in the composite industry.

6.7.2. State of the Art

Nowadays, technology is devoted to the development of new materials able to satisfy specific requirements in terms of both structural and functional performances. The need of exploring new markets in the field of polymeric composites has recently driven the research in Europe towards the development of new products and technologies. In particular, activities on thermoplastic based composites and on composites based on natural occurring materials (environmentally friendly, biodegradable systems) have been of relevant interest in many European countries.

Since the beginning of the 90's years, U.S. and Japan have recognized the need of expanding composite applications. In the field of materials, Japan put more emphasis than U.S. on thermoplastic and high temperature resins. Moreover, due to the large extent of the textile industry in Japan, textile preforming is significantly more advanced than in U.S, and this could lead to the development of cost-efficient automated computer-controlled looms for complex textile shapes. In contrast to the U.S. approach of developing computational models to better understand manufacturing processes, Japanese manufacturing science appears to reside in experienced workers who develop understanding of the process over long period of time. However, Japanese process and product development methods are based on concurrent engineering methodology, which is based on the integration of product and process design.

Biomedical is another important field where composites are applied. Materials, able to simulate the complex structural properties of the natural tissues, which are composite in nature, have been developed but there are still few

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applications. This is due to the delay in the technology transfer from different areas (composite industry and biomedical) and to the lack of cross-disciplinary strategies. In this field, U.S. maintain a leadership role but major centres exist in EU and Japan. Japan recognized the necessity of establishing a "National Institute for Advanced Interdisciplinary Research" which is devoted to research on subjects combining elements from various fields that cannot be adequately treated within the bounds of traditional divisions of science. Among other topics, soft and hard tissue engineering are considered of relevant interests. Tissue engineering activities are growing, as well and strong R&D programmes are present in EU and Japan, even though U.S. have a leadership role in the field.

6.7.3. Trends

The main trends in the structural composite field are related to the reduction of the cost which cannot only be related to the improvement in the manufacturing technology, but needs an integration between design, material, process, tooling, quality assurance, manufacturing. Moreover, the high-tech industry, such as telecommunication, where specific functional properties are the principal requirements, will take advantages by the composite approach in the next future. The control of the filler size, shape and surface chemical nature has a fundamental role in the development of materials that can be utilized to develop devices, sensors and actuators based on the tailoring of functional properties such as optical, chemical and physical, magneto-elastic etc. Finally, a future technological challenge will be the development of a new class of smart composite materials whose elasto-dynamic response can be adapted in real time in order to significantly enhance the performance of structural and mechanical systems under a diverse range of operating conditions.

Over the long period term, U.S. and Japan believe that advances in the materials area would prompt new breakthroughs in the area of composites. In fact, the current emphasis is on "fourth-generation" materials, i.e. those that are designed by controlling the behaviour of atoms and electrons, and which provide carefully tailored functional gradients.

6.7.4. Expectation and Needs for the Next 10 Years

The composite materials market is expected to expand in areas where costs are today a strong limitation. The improvement of the mature manufacturing technologies will benefit from integrated approach where product and process requirements are set at design level. The expected reduction of manufacturing costs of the structural composites will expand applications of such materials to large-scale markets such as civil and goods. Among the paramount needs are large-scale sponsored demonstration project; large scale and long-duration tests programmes; development and support of product certification and specification protocols. In particular, it is demanding to expand basic and applied research in the fields of materials systems for homes, more durable materials to replace aging pipelines and transmission systems, enhanced safety systems for lighter automobiles made from composites, as well as research into even more rapid manufacturing processes, improvements in material handling and storage, and better, more durable and ever more benign resins.

Significant breakthroughs are expected in new composite materials especially in those applications, such as electronic, optic and biomedical, where functionality is the most relevant technical need. Relevant development will be expected in the area of nanophase material synthesis and nanocomposite manufacturing technology. However, further optimization studies are required to implement large-scale production.

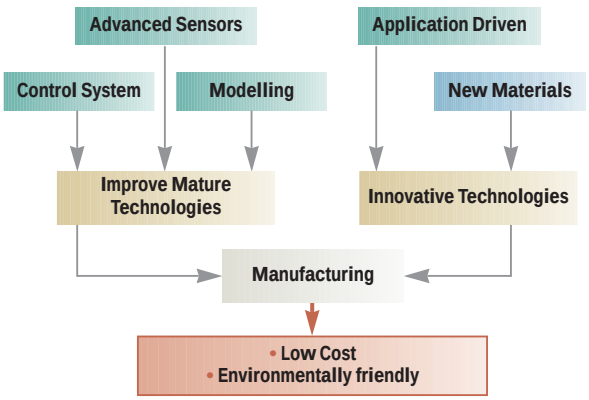

Fig. 6.11. Main trends and expected breakthroughs (yellow) in the manufacturing of composite materials.

Particular emphasis should be devoted to the R&D of composite materials able to respond to dynamic variation of the operative conditions. Smart materials will provide the nervous systems, the brains and the muscles for the existing advanced materials and structure that, at the moment, are a mere skeleton compared with the anatomy forecasted in a near future. Applications are expected in fields of sensors, actuators, and biomedical.

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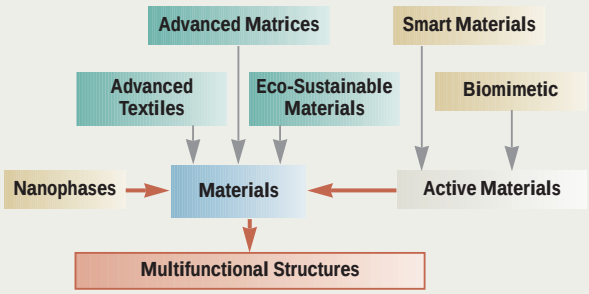

Fig. 6.12. Main trends and expected breakthroughs (yellow) in composite materials.

The quality of human life would be greatly improved by the availability of artificial prostheses (bone, muscles, cartilage, and soft tissues) and organs able to restore, repair or replace structural and functional performances of the natural tissues. The composite structure of the natural systems with its intrinsic complexity needs to be reproduced. Tissue Engineering is one of the major focuses of biotechnological research today, with the expectation that this type of biohybrid technology will ultimately transform the practice of restorative clinics. The approach combines the principles of biology, material science and engineering to culture cells, also heterogeneous groups of cells, using polymeric biodegradable scaffolds as delivery vehicles for cell transplantation to obtain complex three-dimensional cellular constructs. Composite materials should be properly designed to provide anisotropic and/or active scaffolds able to control the cell growth in the reconstruction of complex natural structures.

The expected development of the aforementioned fields needs a serious interdisciplinary approach. As already recognized by U.S. and Japan, significant advancement in the next 10 years in the field of a) functional and structural composites through nanotechnologies, b) smart materials and c) composite for biomedical applications requires cross-disciplinary strategies that should be addressed by combining various scientific disciplines. The available huge amount of human and economic resources, spread all over Europe, should be better coordinated by the creation of new interdisciplinary European research centres that could face the world scientific and technological challenge in these strategic fields.

6.7.5. Conclusions

Research activities, aimed to expand the applications in composite industry, must be addressed to improve manufacturing composite technology, through a better integration of product and process design; to develop new constituent materials with better performances and/or for the tailoring of structural and functional properties for special applications and for the development of new processes and new manufacturing technologies.

Expected breakthroughs are related to the development of multi-component materials with anisotropic and non-linear properties, able to impart unique structural and functional properties. Applications include smart systems, able to recognize and to adapt to external stimuli, as well as anisotropic and active composite systems to be used as scaffold for tissue engineering and other biomedical applications.

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6.8. Electronic Systems

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6.8.1. Introduction

Electronic, photonic, and magnetic materials and systems are at the heart of today's technology revolution and are extremely fertile fields of research. Despite major advances in our understanding and applications in these systems, many basic scientific questions remain unanswered, and we continue to experience remarkable breakthroughs on a regular basis. With increased scientific understanding, we have been able to exploit electronic, photonic, and magnetic materials and systems for amazing technological advances. These technological advances lead in turn to powerful research tools that enable us to advance our scientific understanding of these complex systems, as well as other areas of materials, physics, and chemistry and diverse fields such as medicine, and to enable new fields such biotechnology.

Perhaps more than in any other field advances in our basic understanding and control of semiconductor, optical, and magnetic materials and phenomena enable the technology that underpins today's so-called Information Age. With the continuing decrease in feature size of since the invention of the integrated circuit (IC) more than forty years ago, and the associated increase in transistor density and IC performance, the silicon IC has enabled the computing and communications revolution. "Moore's Law," the projection that the number of transistors per square centimetre of Si would double about every 18 months [1], has guided advances in this technology. Massive research and development efforts have enabled increases in the productivity of the Si IC at a historical rate of 25-30% per year, making low-cost computing widely available.

In addition to the Si IC, major advances in communication bandwidth and associated reduction in cost were also required to enable the Information Age. Advances in fibre optics, introduced into communications about 20 years ago, greatly enhanced communication capability. Communication bandwidth is increasing at an accelerated rate with our increased understanding of optical materials and phenomena. Equally impressive is the advance in the rate of development of other optical components to permit the use of photons to perform an increasing number of functions that were performed by electrons.

In addition to silicon semiconductors, compound semiconductors play a major role in information technology. Compound semiconductor diode lasers provide the photons for optical communication as well as for optical storage and compact disc technology. High performance compound semiconductor diode lasers modulated at gigahertz (GHz) frequencies send information over the fibre optical networks. Very high speed, low power consumption compound semiconductor electronics are key to wireless communication, especially for portable units and satellite systems. Compound semiconductors also offer an extremely fertile field for advancing our understanding of fundamental physical phenomena.

Another key enabler of the information revolution is low cost, low power, high-density information storage that keeps pace with the exponential growth of computing and communication bandwidth. Low cost, high-density storage is provided by magnetic, and to a lesser extent optical, media. Today's highest performance magnetic storage devices rely on giant magnetoresistance in atomically engineered materials.

6.8.2. State of the Art in Electronic Materials and Systems

(a) Silicon-based systems

Transistors with gate-lengths less than 100 nm are under development for high volume manufacturing by leading-edge semiconductor companies. In addition, functioning transistors with gate lengths below 20 nm have been demonstrated. The steady decrease feature size and associated decrease in cost per function has created literally hundreds of applications for silicon ICs. Based on the International Technology Roadmap for Semiconductors [2], industry expects to manufacture integrated circuits with gate lengths of 20 nm by 2014 (Fig. 6.13), which will require significantly greater scientific understanding and control of semiconductor materials and manufacturing processes than are available today.

Silicon-germanium (SiGe) and silicon-on-insulator (SOI) have demonstrated performance superior to transistors and circuits based on bulk silicon and are in volume manufacturing; however, a transition to either SiGe of SOI will only provide a one-time gain.

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(b) Nanostructured materials

Nanoscopic and mesoscopic systems are larger than atoms but small enough that their properties differ from those of bulk materials. When electron wavelengths in such mesoscopic systems are comparable to the structural dimensions and the mean free path for phase breaking, statistical averaging does not eliminate quantum mechanical phenomena. This behavior has been demonstrated by such phenomena as universal conductance fluctuations. Results can be dramatic when electrons are confined in all three dimensions in structures that enhance the electron-electron correlations to exhibit quantization of both charge and energy. The voltage required to add an extra electron can be used to measure the energy levels of these "artificial atoms." These artificial atoms are large enough to display behavior not observed in natural atoms; for example, the superconducting energy gap in mesoscopic Al structures is quantized.

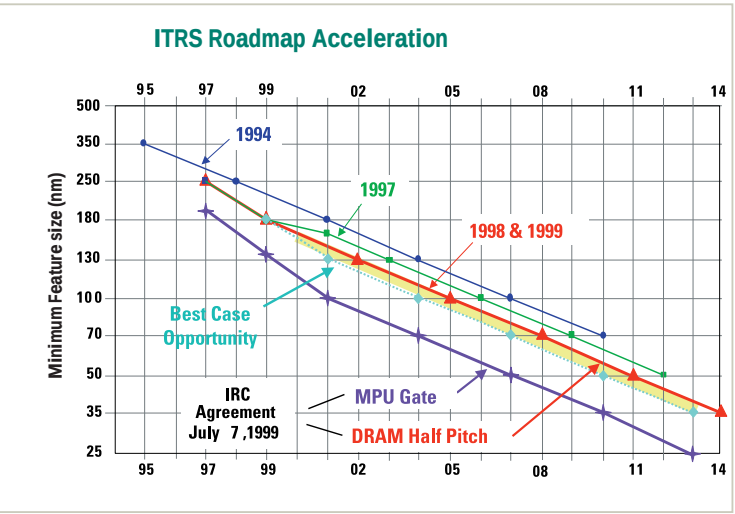

Fig. 6.13. Comparison of the timing of the technology nodes in the 1999 Technology Roadmap for Semiconductors with those in the 1994 and 1997 Roadmaps. The first year for volume manufacturing is listed for two features: isolated gate length and DRAM half-pitch, to accommodate the replacement of memory by microprocessors as the primary technology driver.

In a quantum dot structure, adding an electron to the quantum dot creates a Coulomb field, which repels the addition of another electron. A single electron transistor (SET) can be realized by placing the quantum dot between the input and output channels and adding a control gate. SETs turn on and off again each time an electron is added. The operating temperature of mesoscopic structures increases with decreasing size, and near room temperature operation has been demonstrated in nm-size SETs and Single Electron Memories (SEMs) (Fig. 6.14).

Such devices not only function as transistors, but they also provide insight into the physics of mesoscopic structures. Using the sharp peaks associated with the addition of an electron, the equilibrium ground state energy of the droplet of electrons, as well as some low-lying excited states, can be measured. Other phenomena, such as Kondo behavior, have also been observed in these systems.

In addition to the Coulomb blockade behavior discussed above, resonant tunneling and quantum confinement can be used to create new devices and illustrate new phenomena. In resonant tunneling, the probability for charge carriers to tunnel through barriers is greatly enhanced when the energy levels on the two sides of the barrier are identical. Large changes in tunneling current are realized with small changes in the bias voltage. Quantum confinement structures can be created which serve as electron waveguides, conceptually similar to the waveguides encountered in optical structures. In structures that confine electrons to regions with dimensions comparable to the electron wavelength, quantum interference effects can be used to switch electronic currents.

(c) Compound semiconductors

Compound semiconductors such as GaAs, AlGaAs, InGaAs, SiGe, GaN, GaAlN, etc., offer intrinsically higher speed and lower noise than silicon and have been used to develop very high frequency electronic devices and circuits for microwave and wireless communication applications. Advancing the limits of semiconductor materials technology is essential for increasing the speed of transistors and advancing our ability to modulate light emitting diodes (LEDs) and semiconductor lasers at high frequencies for high-speed optical communication. With more than one element, compound semiconductors offer a wide range of materials and structures with electronic and optical properties that are tailored through band structure engineering.

Band structure engineering through the use of complex heterostructures formed from combinations of semiconductors increases the properties, performance, and potential applications. Heterostructure devices such as heterojunction bipolar transistors, field-effect transistors, semiconductor lasers, and light-emitting diodes are formed from atomic layer control of epitaxial layers with different compositions and thicknesses. The growth of one material on another produces materials not found in nature to create structures with feature sizes comparable to the electron de Broglie wavelength.

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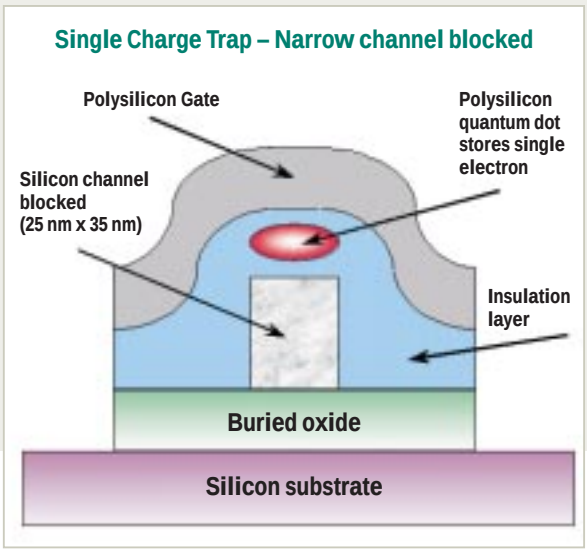

Fig. 6.14. Single electron memory structure based on a polycrystalline silicon quantum dot.

The ability to span the broad spectral region from ultraviolet to long-wavelength infrared was enhanced by the introduction of strained-layer systems. Very high crystal quality layers can be grown for systems with different equilibrium atomic spacing if the thickness of the layer is less than the critical layer thickness at which dislocations nucleate and grow. Such strained (pseudomorphic) thin layers offer an additional degree of control over the electronic band structure of the artificially structured material.

Very high performance High Mobility Electron Transistors (HEMT) were developed by creating nearly ideal two-dimensional electron gases (2DEG) through the growth of modulation doped structures. Today's highest performance transistors, in terms of speed-power product and noise, are pseudomorphic HEMTs.

6.8.3. Future Trends and Research Opportunities in Electronic Systems

(a) Si semiconductor technology

Extensive research will be required to develop new approaches to metal interconnects and new interlayer dielectrics to provide the required IC speed. Cu has replaced Al for the interconnect metallization, and low dielectric constant insulators are being developed to replace SiO_2. While potential candidate materials have been identified for the interlayer dielectric, normal metals can only carry the technology for a few more generations.

Continued scaling of Si technology will encounter fundamental limits as the feature sizes of the transistors become too small to confine the electrons in the channels. In addition, when the information is contained in only a few charge carriers, statistical fluctuations will limit device performance uniformity. Then today's approach to IC technology will no longer be extendable to smaller feature sizes and higher densities, which is stimulating the search for materials and device structures of the future.

Perhaps additional performance improvements for CMOS can be obtained with SiGe on insulator. Ultimately the same fundamental limits will be reached in these materials with continued scaling as with Si.

Major materials-related technical questions for silicon IC technology include: What interconnect technology will be used beyond Cu and low κ – i.e., beyond normal metals and dielectrics – for Si ICs, and how do we manufacture single electron transistors and memories at reasonable operating temperature and cost?

(b) Nanostructured materials

Quantum dot structures are just beginning to be investigated in depth. Circuits are being formed by collections of artificial atoms or molecular electronic structures using such approaches as quantum dot cellular automata (QCA). In today's digital integrated circuit architectures, transistors serve as current switches to charge and discharge capacitors. In QCA, logic states are encoded by the positions of individual electrons rather than by voltages. Such structures should be scaleable to molecular levels with device performance improving with decreasing size. Questions for research include: What are the best approaches to understand and exploit quantum state logic?

In addition to quantum dot-based single electron transistors and memories, nanowires, in which electrons are confined in 2-D, are being investigated for microelectronic applications. Si nanowires can be doped either n- or p-type to transport electrons or holes. Such doped Si nanowires have been used as building blocks to demonstrate diode structures consisting of crossed nanowires and bipolar transistors consisting of heavily and lightly n-doped nanowires crossing a common p-type nanowire. Simple circuits are beginning to be explored using these nanowires. Doped n- and p-type InP nanowires that can function as field effect transistors are being grown.

Carbon nanotubes, which can be formed in either a semiconducting or metallic state, are being investigated for nanoscale microelectronics [3]. Nanowires and carbon nanotubes are ideal building blocks for nanoscale elec-

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tronics. These structures carry charge and excitons efficiently, and field-effect and single-electron transistors have been demonstrated in carbon nanotubes, which can be formed in either semiconducting or metallic states. Such research represents the early stages of exploration of approaches to replace conventional lithographic approaches to patterning semiconducting devices and circuits with an atomic and molecular nanotechnology approach to fabricating devices and circuits.

(c) Compound semiconductors

Controlling the dimensionality of a material on the scale of a few nanometres by growth or processing can greatly alter the density of electronic states (Fig. 6.15) and the electrical and optical properties.

A three dimensional (3-D) distribution of electrons in a metal or semiconductor has a density of available electronic states that increases as the square root of the energy. Enclosing a thin layer of lower band gap material with thickness comparable to the electron de Broglie wavelength between higher band gap materials yields a 2-D quantum well with sharp steps in the electronic density of states. Confining electrons into a 1-D quantum wire produces a series of sharp peaks at the onset of each new quantum mode in the wire, and confining electrons into a 0-D "quantum dot", or a box of size comparable to the wavelength of the electron in all directions, produces a series of even sharper spikes which correspond to a series of confined quantum levels for the electrons in the box. Confining electrons (or holes) in three dimensions leads to giant 'pseudomolecules" with large optical nonlinearities. Such structures can become the basic building blocks for novel devices. One example of a concept that is beginning to receive attention is that of quantum state logic [4], in which a device can be switched between multiple states, in contrast to a field-effect transistor which is either "on" or "off". Excitons, (band-edge bound states between conduction band electrons and valence band holes) have wave functions similar to those of Rydberg atoms. Binding an electron or a hole, or both, in 1-, 2-, or 3-dimensions comparable to exciton diameters greatly affects the excitonic levels and optical properties near the band gap. In theory, 3-D confinement (quantum dots) can produce zero threshold current lasers. Significant research is underway to understand the phase diagram of the excitonic matter in semiconductors and its interaction with photons.

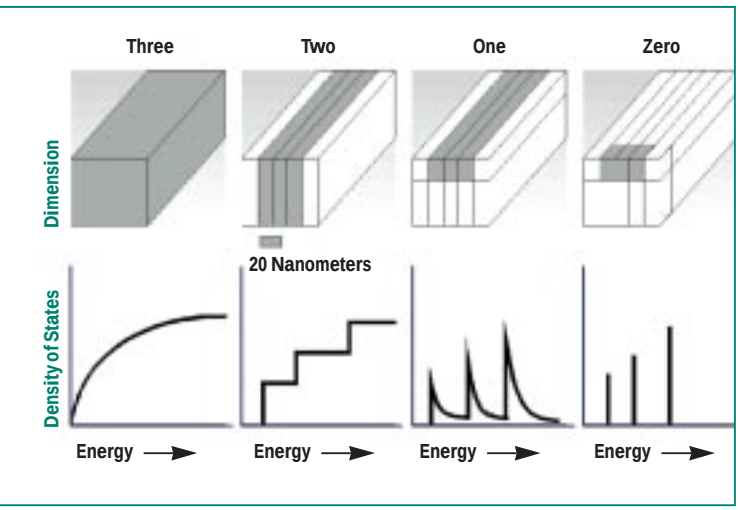

Fig. 6.15. Illustration of the effect of quantum confinement on the density of electronic states (From Scientific American, 8 (1) 26, 1997).

As discussed elsewhere, increased understanding of the physics of quantum microcavities and advances in compound semiconductor growth and processing techniques is also leading to major advances in optical microcavity lasers, LEDs, and detectors.

(d) Organic semiconductors

An emerging and rapidly growing area of research is the synthesis of semiconducting organic materials. Much of this work has concentrated on optoelectronic devices based on electronically active organics, including light-emitting diodes, thin-film transistors, photovoltaics, and nonlinear optical elements. Excitement in this area is generated by the ability to process organics using low-cost methods such as spin casting, micro-contact printing (stamping), and screen printing with the potential to produce large area devices and patterns easily compatible with plastic substrates [5].

The maturest electronics-related application of organic materials is light-emitting diodes. Understanding injection and transport properties that determine current and voltage characteristics are critical areas of research that are advancing rapidly. Organic thin-film transistors with performance comparable to amorphous silicon transistors have been fabricated for switching pixels in active-matrix liquid crystal displays. Improved charge injection and transport are critical to these electronic applications of organic semiconductors.

Another promising area of active organics in electronics relies on the conductivity of doped conjugated polymers. Doped *trans*-polyacetylene, while unstable in ambient conditions, has exhibited conductivity's higher than metals. More stable systems, such as doped polypyrrole, show promise for application as transparent contacts for displays.

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6.8.4. Conclusion

Electronic materials provide an active and growing research area, which continues to yield exciting scientific knowledge and technological advances. Although Si device technology is pervasive, many research questions remain. For example, recognizing that one cannot continue to scale silicon integrated circuits to smaller feature sizes indefinitely raises the question: What is beyond Si? Some of the potential questions to be addressed to answer such questions include: How can self-assembled materials be controlled to create the desired 1- 2-, and 3-D structures? How does one create hybrid structures that exploit the best properties of, e.g., organic or polymeric materials and semiconductors, magnetic materials and semiconductors, or superconductors and semiconductors?

To date much of the semiconductor technology has relied on atomic-level control of crystal growth and lithographic patterning of devices and microstructures. One probable successor to optical and electron-beam patterning for fabricating nanostructures could be atom-by-atom or molecule-by-molecule assembly. Scanning tunneling microscopes have been used to arrange atoms on surfaces and to measure changes in the energies of the surface electrons. Scanning probes have been used to construct single atom switches, in which the movement of an atom from one position to another opens or closes a circuit created by assembling rows of atoms on a surface.

We anticipate a variety of scientific opportunities to emerge from electronic polymers. Potential areas range from molecular electronics, self-assembled nanostructures with giant optical nonlinearities, hybrid structures with organic materials and inorganic quantum dots, and functional polymers that can interface to biological systems. Organic materials will be discussed in more detail in the section on Photonic Systems, since their earliest major impact will probably occur in optical and optoelectronic applications rather than in ultra-high density IC applications.
Significant advances are beginning to be realized in high-resolution ink-jet printing of all polymer thin film transistors and circuits. This approach is attractive both for the low cost of the manufacturing process but also compatibility with a variety of substrates because of the low processing temperatures. Discovering and controlling new self-assembly approaches for low-cost fabrication on structures with atomic-level control are important areas of research that are receiving increasing attention.

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6.9. Photonic Systems

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6.9.1. Introduction

Since the invention of the laser in 1960, a revolution in optical materials and phenomena has stimulated advances on many fronts. This section will focus on two areas to highlight selected advances and opportunities in optical materials and phenomena: semiconductor-based and fibre optic-based materials systems.

The ability to grow devices and structures with atomic layer control in selected materials systems allows the manufacture of high performance, high reliability, compound semiconductor diode lasers, high speed semiconductor-based detectors, billions of light emitting diodes (LEDs) annually for displays, free-space and short-range high speed communication, and numerous other applications. Compound semiconductor diode lasers provide the photons that transport information on optical fibres for telecommunication. Semiconductor diode lasers are also at the heart of optical storage and compact disc technology.
Fibre optics, a relatively recent entrant into the high technology arena, is the preferred technology for transmission of digital information over long distances. In addition to rapid growth in the amount of installed fibre, data transmission rates in a single fibre is increasing exponentially by a factor of 100 every decade.

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6.9.2. State of the Art in Semiconductor- and Fibre Optic-Based Optoelectronic Systems

(a) Lasers and LEDs

We continue to see major advances in optical microcavity lasers, LEDs, and detectors, enabled by increased understanding of the physics of quantum microcavities and advances in III-V and II-VI compound semiconductor growth and processing techniques.

Vertical cavity surface emitting lasers (VCSELS), formed by enclosing an active gain medium between two highly reflective dielectric mirror stacks grown vertically on a substrate, offer major advances in diode laser fabrication and performance. Full wafer fabrication and on-wafer testing offer manufacturing improvements analogous to the manufacturing advances integrated circuits brought to transistors. In addition, the mode pattern and high speed switching performance is well matched to many optical communications applications.

Light emitting diodes (LED) are a closely related area that continues to experience major advances. Improvements in our ability to control the quality and composition of compound semiconductor materials and structures combined with increased understanding of the science and technology have led to dramatic improvements in the efficiencies of red LEDs since the invention of the visible LED in 1960 (Fig. 6.16). The recent development GaN and InGaN light emitting diodes complemented wavelengths of the GaAs/AlGaAs and AlInGaP/GaAs materials systems to provide high efficiency LEDs throughout the visible spectrum [1].

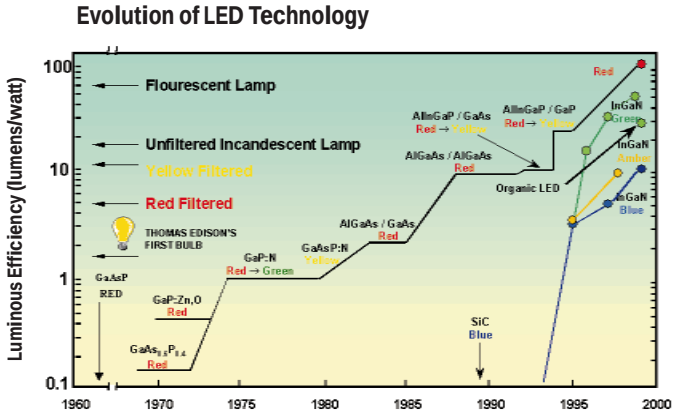

Fig. 6.16. Increase in efficiency and wavelengths available for light emitting diodes in the visible spectral region since 1960 (Courtesy of M. G. Craford, LumILeds).

(b) Organic optoelectronic materials

Electronically active organic materials are an emerging area of LED technology. A variety of organic- and polymeric-based optoelectronic devices, including light-emitting diodes, thin-film transistors, photovoltaics, and nonlinear optical elements are being demonstrated. Organic materials designed at a molecular level will incorporate functional entities with the desired optical, electrical, and mechanical properties that are suitable for cost-effective processing schemes. The vision for semiconducting organic and polymeric materials is large area low-cost devices resulting from inexpensive manufacturing methods like spray painting, ink-jet printing, dip coating, and reel-to-reel processing. Another vision driving organic optoelectronics is the potential for low cost, flexible displays.

Material stability, device performance, and low operating voltage remain important areas of research and engineering, along with understanding injection and transport, which determine current-voltage characteristics. Wide application of organic emitters in display technology requires resolving systems issues associated with electrical drive, patterning, and color fidelity.

(c) Optical data storage

Optical information is stored by forming spots or pits on a reflective surface. The stored information is read by measuring the intensity of the reflected light from a laser beam focused onto the surface. Today's optical recording technology relies on compound semiconductor laser diodes. Diode lasers with shorter wavelengths will increase storage density. Increased optical storage density can also be obtained with stacked semitransparent optical disk layers to produce a 3-D sandwich with laser beams focused on the desired storage layer. The third dimension increases data storage areal density by an order of magnitude.

(d) Quantum dot lasers

Confining electrons in 1-, 2-, and 3-D produces qualitative changes in the density of electronic states and the resulting electronic and optical properties. Research in this nanotechnology area has produced novel structures, including the quantum dot lasers in structures with 3-D confinement and novel electronic and optoelectronic devices in structures with 2-D confinement [2].

Quantum dots, with behavior similar to that of large atoms, are expected to be the basis for future devices. Quantum dots can be formed by a variety of techniques, ranging from patterning an appropriate substrate to self-assembly. Quantum dot lasers with good performance, formed by the island growth that occurs in Stranski-Krastanow epitaxial growth of highly lattice-mismatched systems, were

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first demonstrated in materials systems such as InAs on GaAs. In theory, quantum dot structures can produce lasers with zero-threshold current: all photons generated contribute to the laser action. Defects and distribution in the size of quantum dots limit the performance of lasers with multiple quantum dots in the active region.

(e) Quantum cascade lasers

In conventional semiconductor lasers, light is generated by the recombination of an electron in the conduction band with a hole in the valence band. To first order, the wavelength emitted by the laser is determined by the energy difference between the conduction and valence bands. In a QC semiconductor laser, light is generated by only electrons (or holes) in transitions between two excited states of an ultra thin quantum well. The discrete energy levels arise from size quantization that occurs for quantum well thicknesses comparable to or less than the electron de Broglie wavelength. The active regions of a QC laser are separated by electron injectors that enable electrons to tunnel into the upper excited state of the system. Electrons cascade down an energy staircase, emitting a photon in each active region. N photons are thus created by a single electron traversing an N stage device (N is typically ~ 25), yielding much higher optical power than available in a conventional diode laser at the same wavelength.

The photon energy can be tuned over a very wide range in a given material system by changing the thickness of the layers. Initial QC lasers based on quantum wells in the AlInAs/InGaAs material system demonstrated wavelengths spanning a large portion of the mid-infrared spectrum. These devices exhibit superior operating temperature and optical power performance compared to other semiconductor lasers emitting at these wavelengths. Single mode operation with wide wavelength tuning, as well as active self-mode-locking to produce picosecond pulses, have also been demonstrated. Recently, QC laser wavelengths have been extended to wavelengths beyond 20 micrometres [3].

(f) Photonic band gap structures

Extending the concept of optical microcavities into three dimensions leads to photonic band gap materials [4]. Structures with periodic variations of dielectric constant on a length scale comparable to the wavelength of light alter the propagation of photons analogous to the way semiconducting crystals alter the propagation of electrons, resulting in energy bands for which photon propagation is forbidden. However, a defect in the periodicity introduces localized states in the photonic band gap analogous to the way defects produce localized states for electrons within the band gap of a semiconductor. The nature and shape of the localized states depend on the dimensionality of the defect: confinement in 1-D, 2-D, and 3-D will create mirrors, waveguides, and a microcavities, respectively. Design and manipulation of photonic lattices with such defects promise exquisite control of photons.

(g) Fibre-optic based systems

Optical fibres ushered in a new age of communication. Reduction of transmission losses were accompanied by major advances in electrically modulated single wavelength semiconductor diode lasers operating in the 1.3 and 1.5 micrometre wavelength regions, fast avalanche photodiode detectors, erbium-doped fibre amplifiers and other fibre-based devices, and high power semiconductor diode lasers used to pump the fibre devices.

Invention of Er-doped fibre optic amplifiers enabled much simpler systems. These amplifiers provide modulation format and bit-rate-independent gain over a relatively wide spectral region. They also provide sufficient optical power for high data transmission rates and wave division multiplexing. Fibre gratings formed by exposure to UV light to change the index of refraction in the core of silica fibre doped with germania became building blocks for a plethora of active and passive fibre devices such as filters, amplifiers, fibre lasers, dispersion compensators, pump laser reflectors, demultiplexers, and equalizers.

6.9.3. Future Trends and Research Opportunities in Semiconductor- and Fibre Optic-Based Optoelectronic Systems

(a) Lasers and LEDs future vision

Novel approaches have demonstrated extremely high Q microcavities, including semiconductor-based whispering gallery mode resonators (Fig. 6.17) or droplets of dye solution or polymer in which the index change between the material and air produces a high Q waveguide around the outside of the structure. Such ultra-high Q cavities enormously enhance internal fields to offer new approaches for the study and control of non-linear optical phenomena.

LEDs have long been used in displays, and high efficiency LEDs permit numerous new applications, ranging from vehicle brake lights to highway status and traffic control signs. The higher efficiency and longer life of LEDs result in much lower operating costs compared to incandescent lights. As efficiencies continue to improve, we can expect enormous growth in the areas for application of LEDs; one could envision large area high brightness LED arrays that serve alternatively as a digital television screen, computer display, and room lighting.

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(b) Organic optoelectronic materials

Improved current injection and transport are needed for electrically pumped organic lasers. Hybrid approaches using passive organic gain media optically pumped by electrically pumped inorganic semiconductor lasers are also being explored.

Future research will concentrate on the nanoscience and technology of organic materials, including current flow through single molecules, photochemical modification of a single domain or small arrays of domains, synthesis of materials with giant optical nonlinearities, and integration of organic materials and inorganic quantum dot structures. Such systems hold the promise of materials which self-organize into complex supramolecular arrays. Self-organized 3-D structures may be useful in fabricating photonic band gap structures or color displays [5].

Whispering Gallery Mode Laser

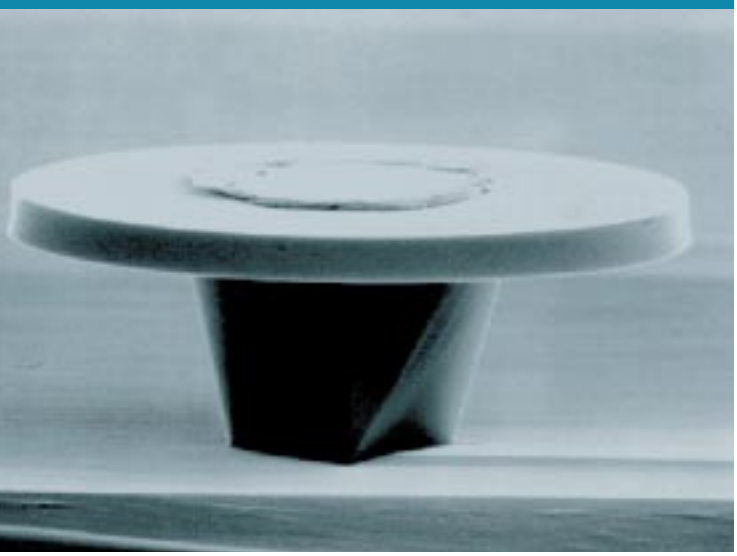

Fig.6.17. Scanning electron micrograph of a very high Q microcavity (Courtesy of Bell Laboratories).

(c) Optical data storage

Approaches to increase the storage density include near-field optical recording and holographic storage. Thousands of holograms can be recorded in a spot of a storage medium with resolution on the order of the wavelength of light. Three-dimensional storage of overlapping holograms promises a projected storage density two to three orders of magnitude larger than conventional optical storage. With the simultaneous transfer of the entire image, holographic storage also promises extremely high data rates.

(d) Quantum dot lasers

Both InAs/GaAs and molecular organic quantum dots are capable of generating single photons on demand, important for quantum encryption. Study of the entanglement of coupled quantum states in closely spaced quantum dot molecules and the creation of structures that combine quantum dot lasers and photonic lattices can be expected to yield new exciting physics and devices. Such coupled quantum dots and structures may become important for quantum computing and information processing [6].

(e) Quantum cascade lasers

Although the first applications based on intersubband transitions was long wavelength infrared detectors, the demonstration of laser action based on such transitions offers the possibility of other optical devices based on intersubband transitions. Intersubband quantum box (IQB) lasers with conventional mirror feedback structures have been shown theoretically to have lower threshold current densities and operating voltages, which should permit higher output power and wall plug efficiencies, than QC lasers.

We can expect other applications of intersubband transitions. Because QC and IQB lasers do not rely on recombination of electrons and holes across the semiconducting band gap, the technology appears to have the potential to be extended to indirect band gap materials, such as SiGe. If such extension is possible, the integration of QC or IQB lasers with Si and SiGe integrated circuits could have a major technological impact.

Approaches to the fabrication of nanowires include growth on stepped substrates formed by cutting a crystal at a small angle to a principal lattice direction and catalyzed growth on selected regions of the substrate. Early work explored the GaAs/AlGaAs system for potential quantum-wire lasers. N- and p-type InP nanowires that can function as field effect transistors can be assembled into p-n junctions that exhibit rectifying behavior and strong light emission to form nanoscale LEDs, and wavelengths smaller than the diameter of the nanowire have been demonstrated. Since the energy states in the nanowires are affected by quantum confinement, the emission wavelength can be tuned by changing the thickness of the nanowires. Such systems may result in one-dimensional lasers.

(f) Photonic band gap structures

Photonic lattices in the near IR and visible spectral regions will offer a radically improved means for controlling light. Essentially zero-loss propagation is predicted, even for a waveguide bend with a radius comparable to the wave-

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length of light. Low cost fabrication of photonic band gap waveguides in the near IR and visible spectral region would enable manufacture and packaging of integrated optical structures to revolutionize integrated optical systems.

(g) Fibre-optic based systems

Enormous strides toward an all-optical network are being made, and the emergence of low-loss graded index multimode plastic optical fibres could lead to a low cost medium to deliver high bandwidth communications over short links from a single mode glass fibre backbone to the desktop.

6.9.4. Conclusion

Major research opportunities abound in optoelectronic materials and devices with today's increased scientific understanding and powerful scientific tools. Research frontiers in the optical area include artificially structured materials with tailored optical properties made by epitaxial growth, lithography, self-assembly, and other techniques.

While the basic physics of charge and energy transfer in organic and polymeric materials is well established, the practical limits to charge photogeneration, injection, and transport are still poorly understood at the microscopic level. Understanding and controlling interfaces between morphologically disordered materials become increasingly important as device dimensions shrink. Developing efficient light-emitting diodes, transistors, and electrically pumped lasers will require good electrical contact to organic materials. Improving material stability is also necessary to make systems based on organic materials commercially viable. Nanostructures based on inorganic and organic semiconductors, polymers, and other complex materials will form the building blocks for future devices and systems.

Research is needed to understand the coupling of exciton-polariton-phonons in nanostructures and quantum cavities, the physics of electro-optical processes in organic materials, and ultra fast non-equilibrium processes in semiconductors, metals, and biological molecules.

Advances in such understanding, along with advances in semiconductor lasers and optical components throughout the visible and near ultraviolet spectral region, will result in numerous technological applications. Other exciting frontiers include integration of quantum wire and quantum dot structures with photonic band gap materials in the visible and near IR wavelength region. Low cost assembly and manufacturing techniques such as self-assembly, stamping, and printing would have a major technological impact.

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6.10. Ecomaterials

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6.10.1. Introduction

The final decade of the 20th Century has been the most important period so far in preparing to create a sustainable society for the century ahead. The United Nations Conference on the Environment and Development named "Earth Summit" was held in Rio de Janeiro in 1992, and the "Rio Declaration on the Environment and Development" and its action plan "Agenda21" were declared to promote practical steps in preparing a sustainable society. In the same year, international standardization on environmental performance, such as environmental management systems and life cycle assessments, were begun to support activities aiming for sustainable development. Just one year before the first Earth Summit, the concept of Ecomaterials (ecologically-benign materials) was proposed to encourage the development of materials that are non-damaging to the global environment and place less of a burden on the planet during production – for example, by being highly recyclable, or by making more efficient use of raw materials.

In this report the challenges facing Ecomaterials are reviewed and classified in order to clarify the next steps in their development.

6.10.2. State of the Art

The concept of Ecomaterials was born through discussions about the future state of materials in the service of humankind and their relation to the environment. Considering the finiteness of the Earth and the biosphere, we should be conscious of the environmental load that our products and materials place on them. Humans produce materials from raw materials taken from the environment to expand their frontiers and make their lives more comfortable. These activities form part of the "human-system", which interacts with the "geo-system" and "bio-system", the latter two systems closely interacting to form the "ecosphere". While the main interest of materials development was traditionally only in the human-system, harmonious co-existence with the other systems has become important in recent years. Ecomaterials development takes a holistic view of the ecosphere and has three strands as shown in Fig. 6.18.

1. Expansion of mankind's frontiers by enabling new technologies.
   This is consistent with the traditional way of developing materials, in which physical, chemical, thermal and/or functional properties are improved and put to use.

2. Harmonious co-existence with the ecosphere by minimizing damage done to the natural environment.
   From the viewpoint of sustainable development, consumption of materials and energy, emission of toxic gases and waste associated with materials processing should be reduced to ease our impact on the resource-circulation system.

3. Optimizing technology and infrastructure to create a healthy life in harmony with Nature.
   Materials should be friendly not only to Nature but also to humans.

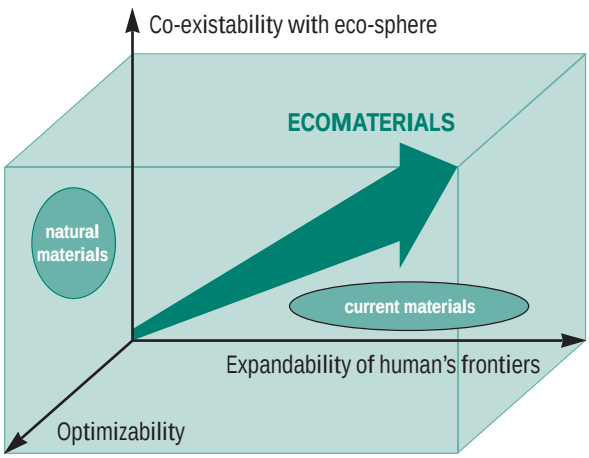

Fig. 6.18. Concept of Ecomaterials

All materials and their properties should be reconsidered from the viewpoint of Ecomaterials; e.g., How can a required property be obtained with less environmental load? How can materials be given improved recyclability? How can maximum performance be acquired with least consumption of materials?

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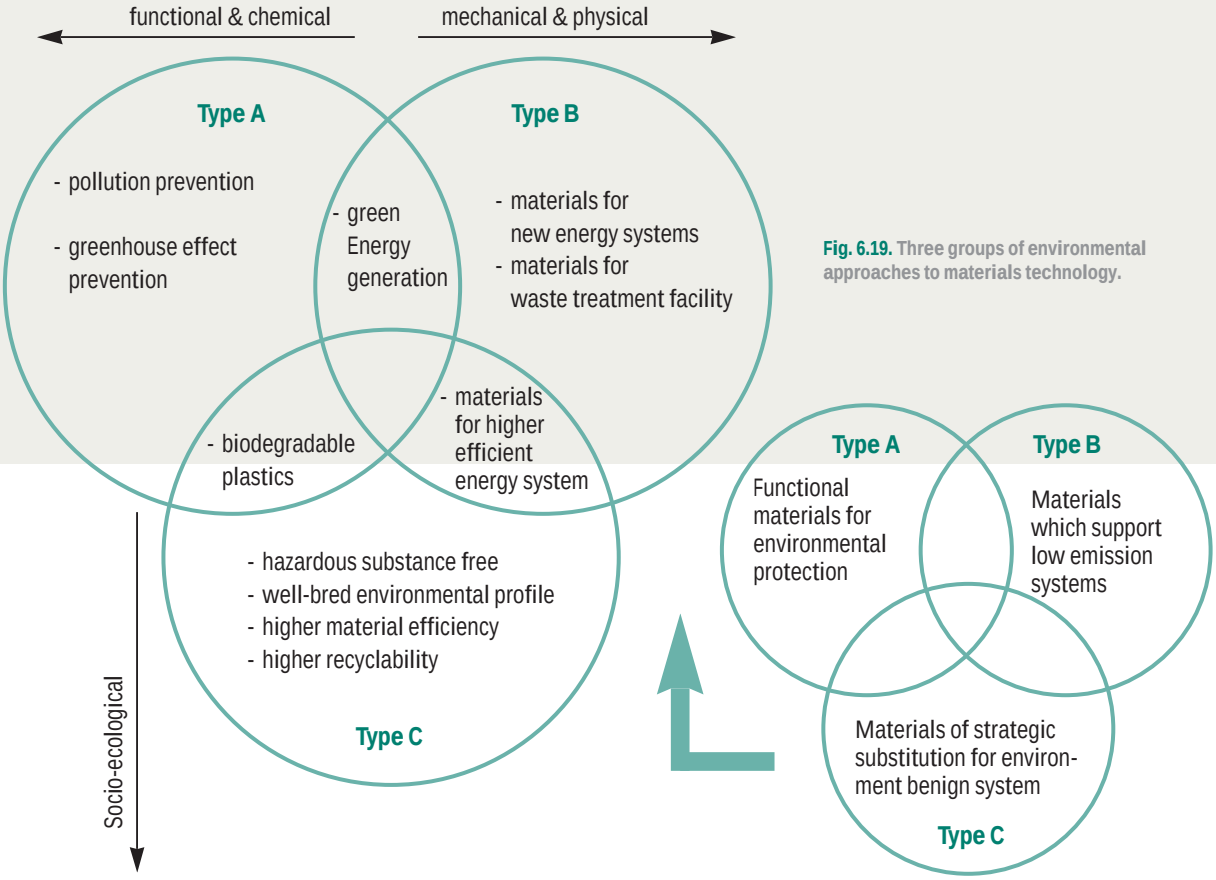

Fig. 6.19. Three groups of environmental approaches to materials technology.

Since the concept of Ecomaterials was proposed, many research projects on materials associated with environmental issues have started in Japan, such as the national research project entitled "Materials design and assessment technology for development of Ecomaterials". Many research groups and courses have been set up around the world, with the result that various Ecomaterials have been developed, and four international conferences on Ecomaterials have been held since 1992.

6.10.3. Expected Breakthroughs

Since environmental issues are world-wide and concern every human activity (the major ones being pollution from mining, acidification by factory and vehicle emissions, the greenhouse effect resulting from combustion of fossil fuels, water pollution, and toxic substances present in waste) fundamental improvements in the materials we use are needed to safeguard the natural environment. The approaches of materials technology to improve the environment cannot be generalized from one viewpoint. They can be divided into three categories based on the relation between a material's properties and its role in improving the environment:

A. Functional materials for environmental protection;
Materials properties are optimized to improve each environmental problem.

B. Materials supporting low-emission systems;
Materials properties are needed to support environmentally benign systems.

C. Materials of strategic substitution for an environment friendly social system;
Materials are used for a given property but society demands that they have lower environmental burden.

These categories are shown in Fig. 6.19.

Catalysts for cleaning up toxic waste, alternative materials to replace toxic substances, CO_2-absorbing substances, and so on belong to the first group (Type A: Environmental Function Type). The second group (Type B: System-Element Type) consists of materials for energy-saving or new energy systems, such as high-temperature turbine blades,

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thermoelectric materials, low-temperature steel pipes for hydrogen transportation, and superconductors. The third group (Type C: Strategic Substitution Type) consists of materials strategically substituted for materials that place more of a burden on the environment. This group is the Ecomaterials in a restricted sense. Ecomaterials have created a new field for materials-designers with the strategic approach of substituting currently-used materials with materials placing less burden on the environment throughout their lifecycles.

The coming paradigm of post-mass production is often called Dematerialization. According to Dematerialization, what one wants is to become aware not of the product itself but of the service mediated by products. In this case, materials can be circulated mainly among producers and service providers. In the coming era, materials technology will become more important, because we have to circulate materials and products with higher quality in an adequate fashion. Materials should be characterized by 1) lower environmental loading, 2) flexibility in production, 3) long life and the possibility of progressive maintenance. These aspects should be maintained throughout the life cycle of the material via a proper life-cycle design.

The requirements of environmentally benign life-cycle design of materials are 1) connection with other industries from the viewpoint of industrial ecology, 2) selection of materials of less environmental load, 3) flexibility for DfE (Design for Environment), 4) no harmful substances after disposal that would make the material a liability after its useful life is over, 5) easy to recycle. These materials will be used as a kind of "material leasing system" which leads us toward a recycling-based dematerialized society.

6.10.4. Roadmap for Future Research

(a) MLCA (Materials Life Cycle Analysis)

Ecomaterials of Type I and Type II have relatively clear targets for development and assessment. A means of measuring the degree of benignity of a material is required. MLCA has to be developed to feed the environmental life-cycle considerations back to materials design. MLCA is developed from LCA to evaluate how well a material qualifies as an Ecomaterial by considering the following differences between a material and its products;

1) The life cycle of a material is different from that of its products. Materials can be used many times by recycling, prolonging the total life cycle.

2) A material has broad generic utilization. The usage stage of a material has wide variations, while that of a product is more specific.

3) Materials properties are sensitive to composition and microstructure.

While materials are classified roughly in LCA of products, differences of composition and of microstructure should be considered in detail to feed back and improve materials design, which is the technology to estimate microstructural/compositional parameters correlated with materials properties.

A database for MLCA also has to be constructed containing representative inventory data of processing of each elemental metal and ferrous alloy. The environmental history, namely accumulated emissions of associated processes from mining to processing, of each alloy and a recyclability parameter will be obtained by accessing this database.

(b) Recyclable materials design

Almost all traditional alloys contain many additive elements to improve their properties. The additives frequently hinder recycling. Traditional materials technology, which has been developed starting from natural resources, cannot treat man-made impurities well. This disadvantage is one of the main reasons for the low cost-competitiveness of recycled material. A new approach to improve recyclability is to control the properties not by element but by structure.

Forming a dual phase steel of martensite and ferrite resulted in improvements in both strength and toughness without adding any other elements. Thermomechanically-treated Al-Si has a dual spherical structure. This structure enables easy forming of recycled Al-Si alloys.

(c) Development of various types of ecomaterials

The development of Ecomaterials can take three approaches corresponding to the way each type of material is to be used. They are classified into four categories from a tech-

Field of diffusive materials

Materials of mass-consumption with useful functions

- **materials without harmful substances in the usage and disposal stages**
  - Pb-free solder, Alternative materials to asbestos, Alternatives to PVC, Plastics with harmless fire retardants, Olefin laminated steel sheet substitute for PVC, etc.

nological viewpoint; 1) harmful substance-free type, 2) low environmental profile type including materials from recycled resources and from natural resources, 3) recyclable materials and 4) materials for efficient energy flow. These approaches have been expanding the area of environmentally benign materials from the stage of "end of pipe" or "mouth of" to the total stages of the life cycle, namely "smart" pipe.

In the field of diffusive materials, where a great amount of materials are consumed daily for the useful function of the material itself, substitution of harmful substances to reduce the environmental burden during and after usage is mainly focused; such as materials for batteries, wrapping, soldering, paints, etc.

As the amount of materials used for construction projects and large-scale infrastructure is enormous, the environmental load "from cradle to grave" of these materials is great. Another side to these materials is their recyclability. Since these materials are relatively easy to manage, the possibility of recycling these materials appears high. The approaches for Ecomaterials in this area are listed in the following table.

Field of high volume materials

Materials for structural use
materials with lower environmental profiles "from cradle to grave"
- materials with less rare materials and with less energy-consuming materials
- materials from nature
  - wood-based materials
  - wood-ceramic
  - soil ceramics
- materials from waste
  - cement from municipal waste (eco-cement)
  - cement from ash
  - various new materials from waste
- circulated materials
  - steel with artificial impurities (tramp elements)
  - reconfiguration of used wood
- materials processed with less emissions and energy consumption

materials with high recyclability
- recyclable designed alloys
  - steels with less number of elements
  - common aluminium alloy
  - alloys robust for impurities
- recyclable designed plastics
- recyclable designed composites
  - ecomposable composites
- composites of same family material

Recyclable designed steel, eco-cement and wood-ceramics are typical results in this field. Recyclable designed steel, which was mentioned before, is not only recyclable but also contains less metallic elements, which are rare and energy consuming to process. Eco-cement is cement made from municipal waste. Eco-cement not only reduces the mining of limestone and other resources but also reduces the waste to be released to the environment after treatment. Wood-ceramic is a new porous carbon material obtained by carbonizing wood or woody material impregnated with phenol resin using ultrasonic vibration in a vacuum furnace. Wood-ceramic has a cellular structure of glassy carbon, which provides good heat resistance, thermal-shock toughness, small thermal expansion, chemical stability, many infrared effects, and so on, without using many man-made materials such as advanced ceramics or plastics.

Field of energy transmission materials

Materials for power generation and transmission
(the major environmental burden is generated at the usage stage in the life cycle)
- materials with higher performance in the usage stage
  - high-strength steels for automobiles
  - heat resistant alloys for high temperature turbines
- light weight alloys for vehicles
  - Al alloys for automobiles
  - Mg alloys
- other materials designed for LCA oriented usage

The third field is that of materials related to energy transmission, transportation and so on, namely those related to energy consumption at the usage stage. Effective property design of materials is used in the development of materials for power transmission media. For example, high-tensile steel sheet reduces the weight of automobiles by 4% resulting in 1.2t less CO_2 being produced during the life-cycle of a car in Japan.

6.10.5. Positions in Japan, the U.S. and Europe

International conferences on Ecomaterials have already been held four times. Last year an Ecomaterials symposium was held in Ottawa, Canada. The 5th conference will be held on 2-5 October this year. In the U.S., the NSF produced a report on research into "Environmentally benign manufacturing". The Industrial Ecology group has held two meetings, and the next meeting is planned for the Netherlands this November. As a practical international

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collaboration, the "Handbook of Ecomaterials" is in preparation with the cooperation of many researchers from Europe, Japan, Canada, U.S., China and others.

In 1999, VAMAS (The Versailles Project on Advanced Materials and Standards) approved an initiative on environmental standardization activities for materials technology entitled "Definition of a Role for VAMAS Participation in Environmental Standardization Activities for Materials Technologies". International collaboration in Ecomaterials research is expected to be promoted more and more in order to find ways of solving materials problems and establish a sustainable society.

6.10.6. Conclusions

In this paper, the state of the art, expected breakthroughs and a roadmap for Ecomaterials research were described. More fundamental research and new ideas are needed in order for these materials to receive widespread use in the near future.

Conclusions

Firstly it should be recognized that having knowledge of potentially advantageous intrinsic properties of a compound/alloy is one thing, but that converting this knowledge into a viable, i.e. practically useful processing route is another thing, which often proves to be extremely difficult, if possible at all. This leads to the following first main conclusion:

- *Whereas significant attention can be paid to the design/prediction of new materials, the major effort should be devoted to the development of successful processing routes.*

Considering, as an example, metal-alloy production, it is clear that the treatment starting with the casting of the raw material and continuing with a combination of heat treatment and deformation, is all-decisive for realizing the properties sought for. This treatment defines and optimizes the internal structure, the so-called microstructure, in terms of atomic arrangement and morphology of the constituents. In other words:

- *Control of the microstructure is the key to successful materials processing.*

In this sense, reviewing the state of knowledge in all material classes of some significance, it is concluded that

- *More basic, fundamental knowledge on processes controlling the microstructure (grain morphology and size, phase constitution, texture, stress) is imperative. Lack of such knowledge is the limiting factor on progress in virtually every area of modern materials engineering.*

This holds for the production of thin films and the area of surface engineering in general, as well for the production of all kinds of composites and bulk materials, both inorganic and organic. To summarize the current impression: it is felt, in contrast with what one may naively presume, that:

- *The gap between fundamental knowledge and technological application has increased in recent years. Hence, basic science on model systems for practical materials should be promoted.*

Control of the mechanisms prevailing on the atomic and molecular scale is necessary, but also on a larger length scale the course of a transformation/reaction should be described quantitatively. For example, quantum mechanical calculations on the molecular scale can be useful, but on a mesoscopic length scale (i.e. at lengths of the order of the size of a crystal grain) for example continuum mechanical calculations (on the basis of finite element approaches) have to be performed.

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Special emphasis today is placed on small-scale structures: thin films and nanoparticles. The synthesis of nanoscale materials is more an art than a science; "nanoresearch" is often conducted on ill-processed materials. This is a recurrent theme in the contributions on thin films, inorganic materials, ceramic materials and composites contained in this chapter. Again, the role of the microstructure must be emphasized in this context: one of the unsolved problems encountered in the sintering of nanosized particles is the preservation of the extremely small grain size in order to maintain favourable (mechanical) properties. The key to progress in these areas is better materials processing.

Expected breakthroughs in the field of materials processing can of course be formulated as the breaking of the barriers which obstruct what is not possible at present. Examples can be found in the contributions of this chapter. Yet, it should be recognized that real breakthroughs in both science and technology very often occur unplanned and are frequently not the aimed-for outcome of a correspondingly dedicated research strategy. Therefore:

- *Although materials processing is naturally strongly related to applications of materials in practice, a substantial part of the research in this area should be curiosity driven and not application driven.*

As specific focal points of interest one may indicate:

- *A (perhaps the) major development in materials processing will be defect elimination and cost reduction (this holds particularly for composites).*

- *The trend will be to niche markets for materials with tailored properties (e.g. development of multicomponent, possibly functional gradient materials often with anisotropic and non-linear properties).*

It may be advantageous to aim for a European centre of excellence on materials processing. The background of this remark is the recognition that it can hardly be expected in the near future that single institutions will possess the full range of, for example, thin film technologies and composite materials processing techniques. Also, concentration of expertise on materials processing can accelerate progress in research in this area. However, it should be noted that in order to achieve genuine understanding of the mechanisms underlying the processing of materials, basic understanding of the reactions and phase transformations involved is required. This, then, would be the focus of the research in other centres of materials science. Therefore a centre on materials processing may best be a virtual one, composed of a number of research groups in Europe which have intimate contact. This form of organization brings about the necessary cooperation and availability of techniques for all researchers in the groups who take part in the centre and it encourages cooperation with materials scientists not participating directly in this centre, who investigate the basic aspects of the reactions and phase transformations of the materials of interest.

As a final remark it is observed that environmental aspects are important as well. This is partly more a political matter than a scientific one. Once society has expressed certain demands, science can contribute. This leads to additional constraints on the conditions for a successful materials processing route, without altering any of the conclusions above.

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7. Advanced Analysis of Materials

Introduction

Advanced materials science is striving for the design of dedicated materials and dedicated materials systems with tailored and often optimized properties. As a prerequisite this task requires detailed information on the microstructure* of a given material (or materials system) on all length scales ranging from atomistic sub-Ångstrøm to macroscopic dimensions. On the other hand the characterization of properties (mechanical, electrical, magnetic, and chemical) must be possible with high accuracy and reliability. One important aspect of materials science is to correlate the microstructure to the properties of a given material (or materials system). One essential task of Basic Research in Materials Science is, in fact, to unravel such laws and relationships in condensed materials and reveal theoretical model for the rationalization of the structure-property relationship. With such rigorous or sometimes empirical structure-property relationships available new materials (or materials systems) can be conceived in applied materials science for advanced novel devices.

Progress in basic research in materials science is, thus, strongly dependent on the development of powerful analytical techniques which provide us with all necessary structural and microstructural information. From a fundamental point of view a material is characterized by its atomic and electronic structure, with this in hand, advanced theories would, in principle, be able to predict as an example, its mechanical or dielectric response. In this chapter we primarily focus on the fundamental analytical techniques which are often based on large-scale facilities and thus depend on a sustained European science policy.

Traditionally, three different analytical approaches are distinguished for the characterization of the microstructure: diffraction, microscopy (imaging) and spectroscopy. Analysis by X-ray and neutron diffraction provides an average structural information. The diffraction techniques are most sensitive to long-range correlations within the material where the dimension of the correlation length should exceed the dimensions of the X-ray (neutrons) beam. Complementary, microscopy imaging yields local information with high spatial resolution which reaches sub-Ångstrøm resolution. The electron microscopy techniques are, therefore, most suitable for the determination of the (local) structure of lattice defects such as dislocations and grain boundaries. By spectroscopy elementary excitations can be investigated in the materials, such as the electronic band structure, phonons or magnons. Again spectroscopy within a transmission electron microscope (analytical electron microscopy) provides those entities with high spatial resolution.

In the last two decades unexpected breakthroughs in X-ray-diffraction and -spectroscopy have been achieved with the availability of highly brilliant synchrotron radiation sources which provide the user with an X-ray beam which

*The term "microstructure" is used in the sense that it encompasses descriptions of the structure of all phases in the material itself and of all lattice defects present in the material, e.g. interstitials, vacancies in non-thermodynamic equilibrium, dislocations, domain boundaries, grain boundaries and interfaces.

◀ Microstructure of a SiC ceramic (transmission optical micrograph obtained with polarized illumination, U. Täffner, MPI für Metallforschung Stuttgart).

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can be tailored in size, energy, coherence, polarization and time structure. The prominent European source is the European Synchrotron Radiation Facility (ESRF) in Grenoble which has started operation in 1994. Comparable X-ray sources are the Advanced Photon Source (APS) in Chicago and SPring-8 in Japan.

Neutron-diffraction and -spectroscopy has developed into a most powerful technique which is complementary to X-rays and particularly useful for magnetic and soft materials as polymers and H-based structures and for the study of the dynamical behaviour of materials. Between the 50s and 70s powerful neutron research reactors have been installed worldwide. The European neutron source, the High-Flux-Reactor (HFR) of the Institut Laue Langevin in Grenoble, has started operation in 1972. Because of the lack of public acceptance and political support of reactor-based neutron sources, one is facing today a neutron draught: Many neutron research facilities have been closed worldwide, today, the new neutron source "Forschungsreaktor München II" (FRMII) in Garching (Germany) is the only new research reactor under construction. One way out of this problem are Neutron Spallation Sources which do not produce nuclear waste and do not suffer from the damaged image of neutron reactors. The European proposal for such a new neutron source is the European Spallation Source (ESS) project which would provide a pulsed neutron beam with a peak power which is factor 100 higher than the HFR allowing access to new dynamic domains in soft and magnetic materials.

In several areas the advantages of X-ray and neutron scattering/spectroscopy are complementary, in some areas they directly compete. Each probe has its strength in the application to different classes of materials. Neutron scattering is well established in the field of polymer science, organic systems and the study of stress/strain states in industrial machine components, whereas synchrotron X-ray scattering still has to find widespread use in the applied community besides its already strong acceptance in protein science and drug design.

It is characteristic for structural as well as for functional materials that their properties are governed by structural feature on various length scales, ranging from the micrometer scale to the sub-Ångstrøm scale. In addition, the time scales which control the dynamic processes and responses of the systems range from several 10^5 seconds to the subpicosecond regime. The analytic control of these length and time scales poses serious challenges to basic research in materials science.

The main drawback of diffraction techniques in materials science has been so far the rather moderate lateral resolution. Information can only be reached with a spatial resolution of several micrometres at best. If, however, the microstructure is non periodic and alters with much smaller length scale (e.g. at grain boundaries, etc.) this spatial resolution is not sufficient for the analysis of lattice defects. Advanced transmission electron microscopy techniques can provide extremely valuable information for the latter problem, for example on the structure, composition and bonding of regions adjacent to lattice defects.

Imaging of materials is a traditional field in materials science. Optical microscopy has been pushed to the limit. By near-field optical microscopy sub-diffraction resolution can be achieved. However, much better spatial resolution can be achieved by electron microscopy. Electron microscopy is an extremely important technique since real materials are mostly polycrystalline and grain boundaries often control the properties (mechanical, electrical) of ma-

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terials. The fractions of "grain boundary volume" to the "bulk volume" is highest for nanocrystalline materials. The properties of grain boundaries control the properties of the bulk. Furthermore, materials are often heterogeneous exhibiting a variation of local structure which may determine the materials properties. This is especially true for three-dimensional nanomaterials where the diameter of the characteristic crystalline feature is only a few nanometres in size.

Imaging of materials on all interesting length scales is possible by advanced instrumentation ranging from advanced optical microscopes to scanning electron microscopes, and other surface science instruments, and, especially, transmission electron microscopes. The detailed analysis of localized structures is the domain of high-resolution transmission electron microscopy (HRTEM) which provides structural information of materials at the atomic level.

Recent revolutionary instrumental developments in HRTEM resulted in the availability of corrector elements which allows to overcome fundamental aberration of electron optical imaging systems. It is expected that the structural analysis of lattice defects and even non-periodic materials can be done with extreme precision of the (average) position of individual atoms or – in crystalline materials – of columns of atoms. Local spectroscopic information from regions about 1 Å in diameter can be retrieved from electron energy loss spectroscopy (EELS) investigations. These measurements result in a better understanding of the variation of local properties within a material. It should be achievable to probe and locate the weak links of materials. It is essential for the further development in Europe that such instruments are available in specific centres and different laboratories. Owing to the complexity of the instruments the specimen preparation technique and the interpretation of structural as well as spectroscopy information requires a real and/or virtual network within Europe, and, especially a number of Centres of Excellence.

NMR is particularly powerful for the analysis of the local structure of noncrystalline materials, as amorphous materials, liquids and biological materials. For the atomic-resolution imaging of surfaces scanning tunneling microscopy (STM) and atomic force microscopy (AFM) are used nowadays in a somewhat routine way, though, the reliable quantitative interpretation of STM and AFM images is still an art which needs experience and training.

Over the last 40 years the control of coherent radiation as provided by lasers has rendered visible and infrared light into a most powerful tool for scientists and technologists. Today coherent light is available with terawatt peak power and femtosecond pulse structure revolutionizing science as a whole, but also advancing into many technological and medical areas. Femtosecond laser spectroscopy allows one today to obtain a realtime insight into the dynamic behaviour of the electrons in materials which opens up a new field of electron spectroscopy. The investigations of structure and function of new materials by ultrafast techniques, nanooptics and a combination of both will be a central topic of future basic research. In addition to the analysis of ultrafast phenomena, optical control of ultrafast processes may become an important issue for realizing specific functions. Simultaneously, technological applications in optoelectronics and information technology are driven by the need for higher data transmission rates and faster information processing, requiring all-optical techniques for modulation and switching. Material processing with ultrashort pulses represents another promising field of application.

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7.1. X-Rays (Synchrotron Radiation)

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7.1.1. State of the Art

Photon beams play an increasingly dominant role in the characterization of materials from the atomic to the macroscopic scale, with the photon spectrum ranging from the far-infrared to the very hard X-ray region. This is particularly so, since the construction of many dedicated synchrotron-radiation facilities in most of the technologically advanced countries in the eighties, and especially the appearance of third-generation synchrotron-radiation facilities in recent years, has enormously expanded the classical means of characterizing materials. Since we are now at the threshold of introducing even fourth-generation sources, namely the free-electron X-ray lasers, this progress will continue, and eventually lead to a merging of laser-based and synchrotron-radiation-based methods in materials research.

The present situation in the field of synchrotron-radiation research in Europe in comparison to the U.S. and Asia can be described as follows: Europe has played a leading role in the development of the field, starting from the pioneering work at DESY in the early seventies, the construction of early dedicated XUV-sources, like BESSY and ACO in the eighties, up to the creation of more modern third-generation synchrotron-radiation sources in the nineties, like ESRF, ELETTRA, MAX II, BESSY II, and the Swiss Light Source. Europe is again leading in the construction of free-electron X-ray lasers, like the TESLA Test Facility at DESY, Hamburg, and there are further new facilities in various European countries in planning and under discussion, in particular those in England and France. In Europe more than 10 000 scientists and engineers make use of synchrotron radiation at different locations shown in Table 7.1.

Synchrotron-radiation based research is very often basic-science oriented, and even though there is a great potential for applied research, this section has often been neglected. The reasons for this are manifold, at least partly based by the rapid methodological progress of the field, which again is a consequence of the rapid progress in the performance of synchrotron-radiation facilities. The rapid progress makes it particularly difficult for industrial companies to keep pace with the fast development of the analytic potential of this field. In contrast to the wide spread opinion of industrial managers, it is not complicated to gain access to synchrotron facilities. At these facilities one is aware of the great industrial potential one wishes to integrate. Applications and remuneration usually come into consideration only when commercially relevant data are provided. Fig. 7.1 shows the European Synchroton Facility (and the High-Flux Neutron Reactor) in Grenoble.

Fig. 7.1. ESRF (European Synchrotron Radiation Facility) and High-Flux Neutron Reactor of the ILL (Institute Laue-Langevin) in Grenoble, France (courtesy ESRF, Grenoble).

7.1.2. Methods

For space reasons, we can mention only a selection of the various synchrotron-radiation-based methods for characterization of materials that have been established to high levels of perfection at different laboratories. They provide information on the spatial structure of the materials, on the chemical and electronic structure, on microstructure, on magnetism and on the properties of surfaces, interfaces, thin films and multilayers. The investigations allow extreme variations of the sample environment, from low to high temperatures and from ultra-high vacuum pressure in the range of 400 GPa.

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Location	Ring (Institute)	Electron Energy [GeV]	Notes
Grenoble	ESRF	6	Dedicated
Orsay	DCI (LURE)	1.8	Dedicated
	SuperACO (LURE)	0.8	Dedicated
	SOLEIL (LURE)	2.5 - 2.75	Planned/Dedicated
Berlin	BESSY	1.7 - 1.9	Dedicated
Bonn	ELSA (Bonn University)	1.5 - 3.5	Partly dedicated
Dortmund	DELTA (Dortmund Univ.)	1.5	Dedicated / FEL use
Hamburg	DORIS III (HASYLAB/DESY)	4.5	Dedicated
	PETRA II (HASYLAB/DESY)	7 - 14	Partly dedicated
Karlsruhe	ANKA (Res. Centre Karlsruhe FZK)	2.5	Dedicated
Frascati	DAFNE	0.51	Parasitic
Trieste	ELETTRA (Synch. Trieste)	2 - 2.4	Dedicated
Daresbury	SRS (Daresbury	2	Dedicated
Didcot	DIAMOND (RAL)	3	Planned/Dedicated
Barcelona	LLS (Univ. Autònoma Barcelona)	2.5	Planned/Dedicated
Aarhus	ASTRID (ISA)	0.6	Partly dedicated
	ASTRID II (ISA)	1.4	Planned/Dedicated
Lund	MAX I (Univ. of Lund)	0.55	Dedicated
	MAX II (Univ. of Lund)	1.5	Dedicated
Villingen	SLS (Paul Scherrer Institut)	2.4	Dedicated

Table 7.1. European Synchrotron Radiation Sources

In structure research, classical powder diffraction can now be performed with an angular resolution that provides enough highly resolved reflections for *ab initio* structure solutions in excess of 30 independent atom positions per unit cell. Crystal sizes can be determined up to 1 µm. Stress and strain analysis with high spatial resolution can be performed on iron-based samples of up to 15 mm thickness. Current efforts in synchrotron-based powder diffraction focus onto the 3D-imaging of strain in single grains exploiting the recent achievements in X-ray microbeams and X-ray focusing.

Element-specific chemical information is obtained from core-level photoelectron spectroscopy and X-ray absorption of near-edge fine-structure (XANES) spectroscopy, since highly monochromatic X-ray and XUV beams can be tuned to the various photon energies of interest. Powder diffraction and XANES spectroscopy allow following chemical reactions in real time with a rate of a fraction of a second. The electronic structure can be determined in k-space using angle-resolved photoemission and X-ray emission spectroscopy with a similar time resolution.

Different aspects of magnetism can be investigated and analyzed in great detail with various magnetic dichroism techniques in X-ray absorption, X-ray reflection, photoemission, and X-ray emission as well as with magnetic X-ray diffraction. Resonances at the X-ray thresholds allow disentangling the individual contributions of the elemental constituents to the total magnetization. Resonant magnetic X-ray diffraction has been pushed to provide magnetic-structure information on ultrathin films with a thickness as low as 10 monolayers. Other powerful methods for the study of magnetic materials include spin-resolved photoemission and nuclear resonant scattering, two methods that benefit a lot from the new intense X-ray beams.

Microscopic techniques such as soft and hard X-ray microscopy, photoemission microscopy (PEEM), X-ray-microprobe analysis, and phase-contrast imaging are developed continuously to better spatial resolution and to a higher accuracy. Resolution limits between 1 µm and 20 nm have been achieved, depending on the technique. Some of these techniques provide also chemical and magnetic contrast. Tomographic reconstruction of composite materials, foams, and inhomogeneous samples can be obtained with 1 µm resolution.

7.1.3. Special Focus: X-Ray Powder Diffraction

X-ray powder diffraction is widely applied for the characterization of crystalline materials. The method has been traditionally used for phase identification, quantitative analysis and the determination of structure imperfections.

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In recent years, applications have been extended to new areas, such as the determination of crystal structures and the extraction of three-dimensional microstructural properties.

The method is normally applied to data collected under ambient conditions, but *in situ* diffraction as a function of external constraints (temperature, pressure, stress, electric field, atmosphere, etc.) is important for the interpretation of solid state transformations and materials behaviour. Various kinds of micro- and nano-crystalline materials can be characterized from X-ray and neutron powder diffraction, including inorganics, organics, drugs, minerals, zeolites, catalysts, metals and ceramics. The physical states of the materials can be loose powders, thin films, polycrystalline and bulk materials.

Phase identification is traditionally based on a comparison of observed data with interplanar spacings, *d*, and relative intensities, *I*, compiled for crystalline materials. The Powder Diffraction File, edited by the International Centre for Diffraction Data (U.S.), contains powder data for more than 130 000 substances. New search/match procedures are based on digitized patterns instead of a list of different values of *d* and *I*, *respectively*.

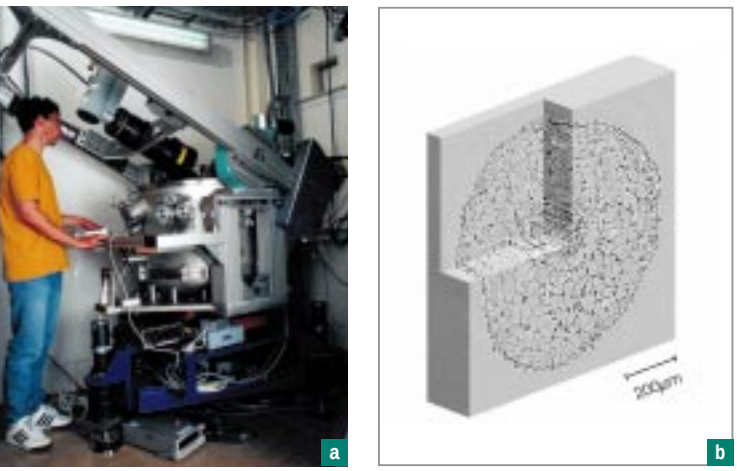

Fig. 7.2. (a) Microfocus beamline ID13 at the ESRF; **(b)** Picture of 3D topography of a metal foam.

Quantitative phase analysis involves the determination of the amounts of different phases present in a multi-component mixture. The powder method is widely used to determine the abundance of distinct crystalline phases, e.g. in rocks and in mixtures of polymorphs, such as zirconia ceramics. Modern approaches are based on the Rietveld method. Because of the potential health hazard of respirable crystalline silica, X-ray powder diffraction is also used for identifying and quantifying silica of all types of samples from airborne dusts to bulk commercial products.

Among the most noteworthy advances of the powder method is the determination *ab initio* of crystal structures from powder diffraction data (to date more than 400 successful examples have been reported). Here the resolution of the pattern is of prime importance. In addition to X-ray sources, neutrons also play an important role in powder diffraction structure analysis, e.g. in case of too low atomic contrasts for X-rays and for precise refinement of atomic coordinates. Neutron powder diffraction was used to determine the oxygen content and position in high T_c superconducting cuprates.

Powerful methods are available for pattern indexing, extraction of integrated intensities, structure solution and refinement of the structure model with the Rietveld method. New direct space methods for crystal structure determination have been introduced, e.g. Monte Carlo simulated annealing, genetic algorithm, crystal structure prediction by energy minimisation and molecular modelling, etc. These techniques are promising approaches, even in case of molecules with several torsion angles. A promising approach is based on combining NMR, electron diffraction and powder diffraction by X-rays.

Microstructural imperfections, such as lattice distortions, stacking and twin faults, dislocations and crystallite size distributions, are usually extracted from the shape of individual diffraction lines. Recently, profile modelling *(synthesis)* techniques have extended the frontiers of microstructural investigations. They include the effect of crystallite size distributions, the effect of lattice distortion parameters and the effect of strain fields in crystalline materials.

Time- and temperature-dependent X-ray diffraction involves the *in situ* measurement of series of diffraction patterns as a function of time and temperature. It is possible to establish the reaction path during solid state transformations and to determine transformation kinetics: e.g. the investigation of fast and self-propagating solid combustion reactions on a subsecond time-scale, using synchrotron radiation for high intensity. The time required for collecting data decreases considerably with the availability of fast detectors, such as position sensitive detectors, and high brightness of modern (Synchrotron) X-ray and neutron sources. Equipment has been developed for *in situ* application of heating, pressure and tensile testing. *In situ* powder diffraction can also be combined with complementary techniques applied simultaneously, such as EXAFS (Extended X-ray Absorption Fine Structure).

Breakthroughs are expected in the following areas:
(i) Microstructure analysis. The precise characterization of the microstructural properties of “real” materials will become possible.

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Synchrotron Radiation Techniques (Selection)	Application; Trends
Micro-beam diffraction	Routine operation down to 2 µm, sub-µm in testing
Magnetic X-ray diffraction	Element specific; film thickness less than 10 monolayers
Powder diffraction	Real time; ultra-high-resolution (see Sect. 7.1.3.)
Anomalous small angle X-ray scattering	Element specific, high-resolution
X-ray absorption fine structure (XAFS)	Element specific coordination shells
High-energy X-ray diffraction	Stress and strain of bulk samples; texture – high spatial resolution, 3D tomography of large samples
Inelastic X-ray scattering	Electronic excitations, elastic response – element specific, small samples, high pressure
Nuclear resonant scattering	Local magnetism at high pressure; small samples
X-ray micro-tomography	Phase contrast imaging; submicron spatial resolution
Time-resolved spectroscopy and diffraction	ρS dynamics of catalytic reactions; fs with XFEL
X-ray microscopy (hard and soft)	30 nm resolution possible; 10 nm envisaged
Magnetic dichroism	High potential for magnetic multilayers
UHV Surface diffraction	Oxidation at catalytic surfaces
XANES spectroscopy	Chemical reactions – element specific in real time

Table 7.2. Recent Developments in Synchrotron Radiation Applications.

(ii) Stress analysis. The analysis of macro-stresses by powder diffraction analysis gives new impulses to understand the elastic and plastic interactions of grains in massive specimens.
(iii) Crystal structure analysis. More complex structures will be solved using more powerful software and methods to be developed in the future.
(iv) *In situ* diffraction. Studies of materials under 'working' conditions and experiencing dynamic microstructural changes will become of paramount importance to understand materials performance

There are many laboratories using powder diffraction on a primitive level. A European network should be developed, with the help of the existing EPDIC (European Powder Diffraction Committee) to train researchers and technical staff in order to perform high-quality experiments and evaluations. EPDIC is organizing a conference series in modern powder diffraction. The International Centre of Diffraction Data (ICDD) is an U.S. organization. Only relatively recently in Europe the European Committee for Standardization (CEN/TC 138) started an extensive project on the use of diffraction methods.

7.1.4. Needs and Trends

X-ray and neutron diffraction at large scale facilities techniques, see table 7.2, are now established through pioneering experiments. Only a few of these novel and powerful techniques find a community, which makes regular use of them as a standard tool in materials research. Even though many of the researchers working on materials become increasingly aware of these methods, many of them need a specific support to access the synchrotron-radiation facilities and to make optimal use of the opportunities provided there.

There are several reasons for the time gap between the development of powerful new synchrotron-radiation-based analytical methods and their actual use in materials research. Besides the rapid progress in the field mentioned above in Sect. 7.1.1, one of the reasons has to do with the fact that many of these new and advanced methods are developed by physicists, while those involved in materials research are mostly chemists or engineers. Therefore, one should bring the two communities together.

Experimental techniques have been pushed to new frontiers already with the introduction of 3rd generation of synchrotron sources. These trends will be enhanced even more strongly with the coming XFEL[1]. Spatial resolution achievable nowadays by microdiffraction and imaging is approximately 30nm with a future limit below 10nm. A combination of spectroscopy and diffraction is going to be applied to all categories of diffraction experiments by moving to the absorption edges of specific elements and enhancing greatly the sensitivity for selected elements even for the smallest sample dimensions. The trend for

1) XFEL: X-ray free electron laser

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time-resolved measurements is now in the picosecond range, but the real need in material science lies in the femtosecond domain, which will be achievable with the XFEL. The exploitation of the coherence of the new sources will set new trends in allowing a simultaneous combination of microscopic length scales with macroscopic ones.

7.1.5. Measures

The measures supported by the European Community to counteract and improve the described situation should have in mind to (i) enhance and spread the knowledge about these powerful novel techniques in materials research in the community and (ii) to ease the access to the facilities. However, the involvement of university groups with their young and dedicated researchers is of crucial importance, because they guarantee progress and will help to counteract stagnation and frustration.

To enhance and spread the knowledge about synchrotron-radiation-based analytical techniques in materials research the following measures are proposed:

• Support of interdisciplinary networks "Application Lab for Analytics with Synchrotron Radiation in Materials Research", which should be administered by a leading research group not directly connected with a synchrotron-radiation facility. Such Application Labs would provide easy access to the most advanced techniques, bringing both application-oriented users and basic-science-oriented researchers together.

• Creation of fellowships for doctoral students and post-doctoral scientists, particularly for students from those European nations that do not possess national synchrotron-radiation facilities by themselves. These fellowships should allow dedicated and gifted graduate/postgraduate students in materials research or solid state science to join leading groups at other European universities and research centres that are heavily involved in synchrotron-radiation research with easy access to beam time.

• Support of special European workshops and conferences with the aim to bring the materials-research and basic-science oriented communities together to exchange the potentials of synchrotron-radiation-based research in materials science and development.

The access to the facilities has to be eased, particularly for non-specialized scientists, who do not want to get too much involved into the techniques, but just want to use them for their development purposes. Special measures have to be taken at the synchrotron-radiation centres themselves. Most centres are presently organized in a way to support only relatively experienced users of synchrotron radiation, a situation that is not very helpful for the use of standardized methods of characterization with high throughput. At specific beamlines of SRC-Daresbury, DESY-HASYLAB and the ESRF industrial users pay for shifts of beamtime and experienced personnel to support them. In order to achieve a similar opportunity for the non-industrial materials science community, the following measures are proposed:

• Support of specific "Local contact for materials characterization" of this community at relevant synchrotron-radiation facilities, staffed with personnel (scientists, engineers) that are experienced both in the use of synchrotron radiation and in materials science. Those staff people of the synchrotron source should be the primary contacts for materials researchers from the different institutions in the European community.

• European measures should be taken in the field of the application of powder diffraction methods to "real" materials.

• A network of tabletop X-ray lasers with XFELs as technology drivers should be developed. This could help to avoid a long timelag between innovation and application as is the case for the established synchrotron sources. The needs of the materials science community should be brought to the attention of the synchrotron scientist at an early stage as input into the development process of new beam stations. The largest impact of LINAC driven X-ray FEL facilities to materials science may well come from the very high peak brilliance in flashes of only 100 femtoseconds duration, which allows to study the time development of non-equilibrium states of matter. Also very specific ways of processing novel materials may come up. Unfortunately it will need probably another 10 years before multi-user facilities up to the needs of the materials science community will be available. In addition, difficult new experimental techniques have to be developed, e.g. pump & probe experiments in the femtosecond time scale, including synchronising the appropriate detectors. Such technical developments can only be successful if laboratory based sources with the proper time structure and sufficient peak flux or brilliance is available for the individual research group. Such equipment will also be most important for preparation of novel experiments finally planned to be performed at the XFEL facility. In recent years tremendous progress has been made in laser technology, especially in higher harmonics generation and with plas-

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ma X-ray lasers, the peak intensities produced are getting close to the needs for materials science as described above. Therefore an EC network focussed on the development of novel approaches to study materials in their non-equilibrium states with X-ray lasers, both tabletop and LINAC driven FELs, should become of very high benefit for materials science as a whole.

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7.2. Neutrons

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7.2.1. State of the Art

Europe operates at present the two premier neutron scattering facilities in the World, namely the High Flux Reactor ILL (Institute Laue Langevin) in Grenoble and the Pulsed Spallation Source ISIS in the UK. Europe also operates 13 smaller local sources shown in Table 7.3. The size of the neutron scattering community in Europe is of the order of 4500 scientists.

Initially neutron scattering was entirely a method exploited and used by physicists. Today instrumentation is available for a much broader usage as it can be seen in Fig. 7.3. A recent survey revealed that about 20% of the users are working in materials science.

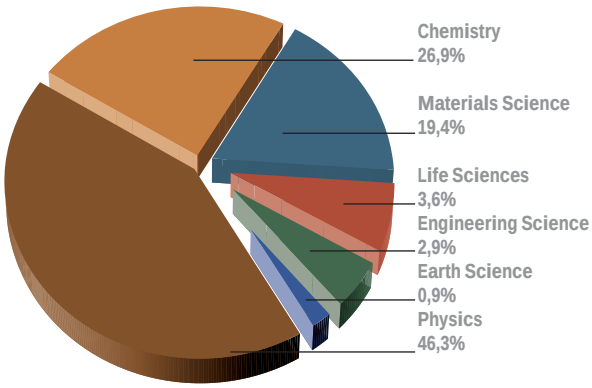

Fig. 7.3. The exploitation of European neutron scattering science across the major scientific and technological disciplines (From the ENSA Survey of the Neutron Scattering Community and Facilities in Europe - an ESF/ENSA publication ISBN 2-912049-00-8, 1998).

7.2.2. Method

Neutrons have a considerable advantage for texture and microstructure studies because they give an accurate bulk average, whereas techniques with small sampling volumes may only sample a few grains.

The production process for certain materials (for example densification in powder metallurgy, precipitate growth drawing of fibres, grain kinetics during annealing) may be studied in real time and *in situ* by scattering methods, in order to understand and control materials processing. The behaviour of materials under operational conditions are another important issue, where problems like the discharge of batteries, ion conduction in fuel cells, the action of catalysts, or aging processes may be investigated. Finally, interfacial properties are gaining increasingly more attention, with broad implications for protective coatings and corrosion, lubrication and adhesion, functional layers, biocompatibility, and other topics.

During the last twenty years, the understanding of soft materials has been significantly advanced by small angle neutron scattering (SANS), combined with labeling through the H-D replacement method, and by neutron spin echo (NSE) spectroscopy, thus facilitating the determination of the properties of substances on mesoscopic length and time scales. Today, SANS is the pre-eminent technique for determining polymer conformations, with important implications for, among others, chain deformation and rubber elasticity, polymer brushes stabilizing colloids, or for chains at interfaces relevant for gluing, etc. Fig. 7.4a shows the experimental setup of a small angle scattering beamline. An experimental result obtained with SANS can be

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Location	Source (Institute)	Power (MW)	Notes
Prague	LVR-15 (NPI, Czech Republic)	10	
Europe	ESS	5	Pulsed source; proposal submitted
Grenoble	HFR (ILL, France)	58	Continuous source
Saclay	Orphee (LLB,France)	14	Continuous source
Berlin	BER-2 (HMI, Germany)	10	Continuous source
Jülich	FRJ-2 (KFA Jülich, Germany)	23	Continuous source
Geesthacht	FRG (GKSS, Germany)	5	Continuous source
Munich	FRM-II (TU Munich, Germany)	30	Continuous source
Budapest	BNC (KFKI, Hungary)	10	Continuous source
Kjeller	JEEP2 (IFE, Norway)	2	Continuous source
Swierk	IAE (Poland)	20	Continuous source
Moscow	IR8 (Russia)	8	Continuous source
Ekaterinburg	IWW-2M (Russia)	15	Continuous source
Gatchina	WWR-M (PNPI, Russia)	18	Continuous source
Dubna	IBR2 (JINR, Russia)	2	Pulsed source (fission)
Studsvik	R-2 (NFL, Sweden)	50	Continuous source
Villigen	SINQ (PSI, Switzerland)	1	Pulsed source
Delft	HOR (IRL, TU Delft, The Netherlands)	2	Continuous source
Abingdon	ISIS (RAL, U.K.)	0.16	Pulsed source (plans for upgrade)

Table 7.3. Neutron Sources in Europe.

seen in Fig 7.4b. Multicomponent systems may be studied by contrast-matching techniques and tasks like the exploration of micro-heterogeneity in multiblock copolymers or interfacial reactions may come into focus. Dynamic experiments with NSE provide insight into molecular rheology.

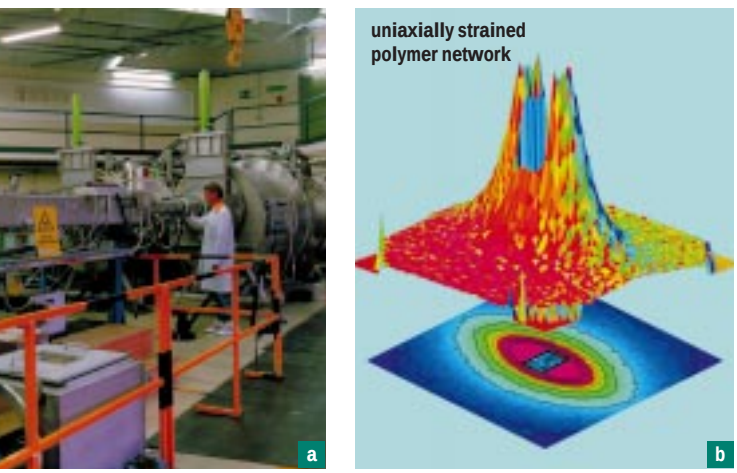

Fig. 7.4. (a) Small-angle neutron scattering beamline KWS2 at the FRJ-2, Jülich, **(b)**Two-dimensional wavevector dependence of the structure factor of SANS yields detailed structural information on global and local topologies on different length scales, ranging from the radius of gyration to the tube diameter or smaller.

Another challenging research field is the self-organization of multi-component systems, like amphiphilics in oil or water, where structural, kinetic and dynamic aspects can be investigated. The response of soft materials to external fields like shear, temperature or pressure, is another area of interest, with clear technological implications, such as an understanding of processing methods such as drawing, spinning, etc. of various materials including rubbers. Complex fluids in confined geometry may be accessed, allowing, e.g., an exploration of techniques for tertiary oil recovery. Neutron reflectometry is the technique of choice for studying the morphology of artificial membranes, interfaces, films, or for studying, among others, lubrication, interdiffusion phenomena and adhesion.

Recently, the application of scattering techniques to engineering problems has drawn much attention with a continous growth. At present the main areas of interest are stress determination in the interior of bulk materials and the diagnostics of material treatment and processing.

From space-resolved diffraction measurements one obtains the stress in the interior of a sample. The knowledge of the stress in machine components (for example, in the vicinity of welds) is important in determining how far the material is from yielding. Another application is the *in situ* investigation of the redistribution of atoms by thermal diffusion, e.g., in a turbine blade. This method can help determine the lifetime of critical mechanical components. The corresponding diagnostic methods are diffraction or small angle scattering. An exciting potential new application would be to use diffraction to follow heat treatment, to optimize the

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thermal treatment process. Stress, as well as the grain orientation, would have to be measured as a function of time in different regions of a machine component. The process of forging could be investigated in a similar way.

The main methods are diffraction, specialized for texture and strain analysis, and small angle scattering. A recent and very attractive development is neutron tomography, for example, for imaging hydrogenous fluids in the interior of machine components, and structural reinforcement of concrete.

Neutron scattering is and will always be an intensity limited technique, and it is the intensity, which in general limits the exploitation of neutron scattering. New instrumentation at existing sources will advance the capabilities in the same way as demonstrated with the third and fourth ring in Fig.7.5. A true leap forward will be the result of the third generation neutron sources. i.e. there will be room for development in all areas of materials science mentioned above. Experiments, which are marginally possible today, will be routine and new areas or more complex systems will be open to neutron scattering with stronger sources.

Neutron Scattering Techniques (Selection)	Application & Trends
Small angle neutron scattering (SANS)	Routinely used in Material Science
Neutron Tomography	Routinely used in Material Science
Magnetic neutron diffraction	Standard method for magnetic structure analysis
Polarized neutron diffraction	Complex magnetic structures; ferromagnetism
Inelastic magnetic scattering	Exchange coupling, magnetic anisotropy
Polarized neutron reflectometry	Magnetic multilayers, magnetic roughness; magneto-electronics, spin valves
Diffraction	Highly sensitive to oxygen, carbon, hydrogen
Powder diffraction	Magnetic samples; light elements
Stress-strain scanning	Routinely used in Material Science
Inelastic neutron scattering (Time-of-flight, Triple-axis, Spin-echo)	Fast ionic conductors; hydrogen storage and sensing; dynamics of polymers and glasses

Table 7.4. Recent Development in the Application of Neutron Scattering.

A compact overview of the very diverse range of science studied with neutrons from the early days in the sixties until today is summarized in the fan of Fig. 7.5.

7.2.3. Trends and Needs

Europe faces the imminent closure of several aging research reactors. The only new facility being built in Europe at present is FRMII reactor in Munich. This reactor will be an optimized second generation neutron source which to a large extend will replace other facilities being phased out. On the other hand the U.S. and Japan are at this moment preparing to alleviate their local "neutron droughts" through major investments in third generation advanced neutron sources, and are thereby posing a very serious challenge to European supremacy in the field. The American SNS source is a 2 MW spallation source, which will be in operation by 2006. The Japanese spallation source is not finally approved yet. In Europe a group of 13 laboratories from 11 countries is preparing a proposal for a 5 MW spallation neutron source ESS (European Spallation Source).

The FRMII reactor in Munich, is urgently needed by the materials science community. A possible long delay of its startup would be very costly both in terms of money and loss of highly qualified personal and user base. Strong support from the EC is needed to overcome the present political hurdles.

In the long-term, a powerful new, pulsed neutron source is needed to keep the strong European neutron science efforts competitive with the U.S. and Japanese efforts.

7.2.4. Measures

It takes 7 to 10 years to build a new neutron source. The cost of a new facility is of the order of 1 Billion €. It is therefore imminent that Europe agrees on building the ESS – a third generation neutron source. With a decision to build the ESS by 2001-2002 - funding for engineering design and prototyping will be needed from 2002-2003 and construction could begin at the earliest in 2003, with an operating source in 2010.

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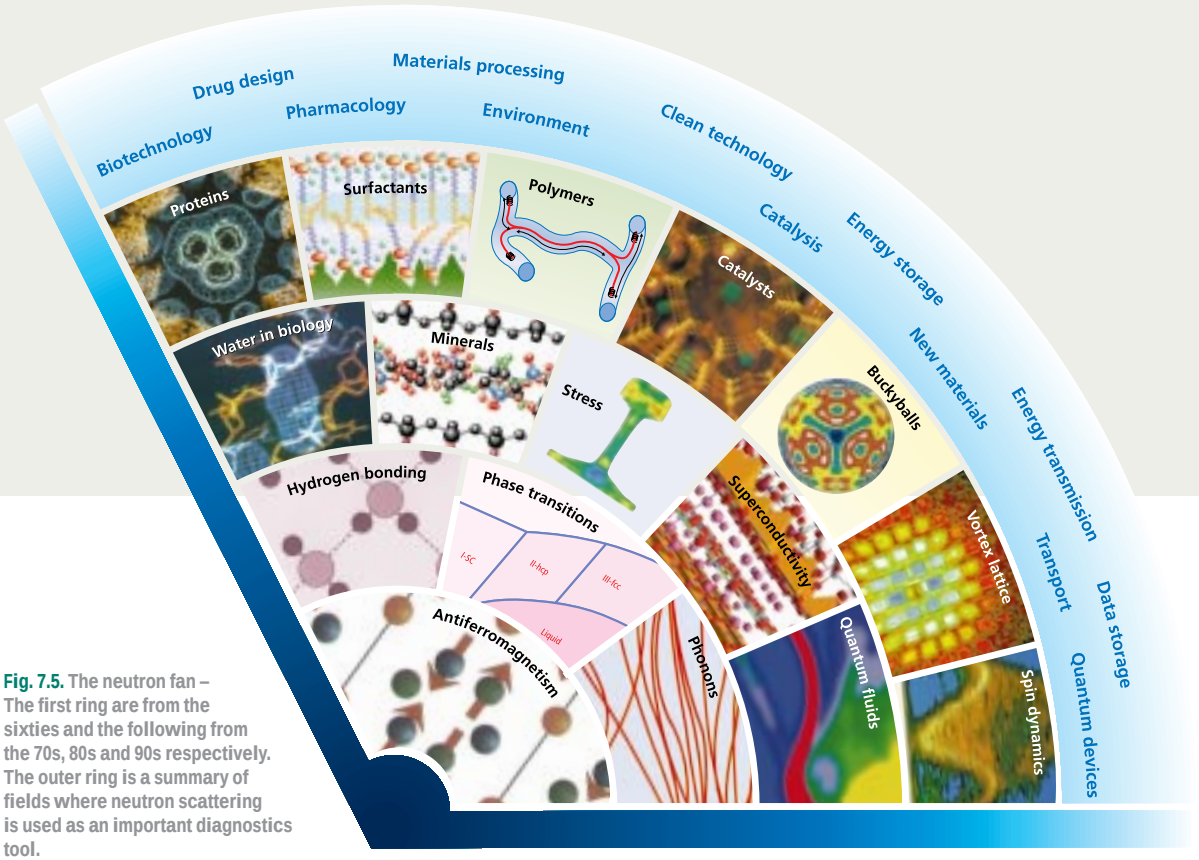

Fig. 7.5. The neutron fan – The first ring are from the sixties and the following from the 70s, 80s and 90s respectively. The outer ring is a summary of fields where neutron scattering is used as an important diagnostics tool.

Other measures supported by the European Community to counteract and improve the described situation should have in mind to (i) enhance and spread the knowledge about the powerful novel techniques in materials science and in the community and (ii) to ease the access to the facilities. However, the university groups with their young and dedicated researchers should be centrally involved, because they guarantee progress and will help to counteract stagnation and frustration.

To enhance and spread the knowledge about neutron-based analytical techniques in materials research the following measures are proposed:

- Support of interdisciplinary networks “Application Laboratories for Analysis with Neutron Scattering in Materials Research”. The laboratory should be administered by a leading research group not directly connected with a neutron scattering facility. Such Application Labs would provide easy access to the most advanced techniques, bringing both application-oriented users and basic-science-oriented researchers together.

- Creation of special fellowships for doctoral and post-doctoral students, particularly for students from those European nations that do not possess national neutron scattering facilities by themselves. These fellowships should allow dedicated and gifted graduate and post-graduate students in materials science or solid state science to join leading groups at other European universities that are heavily involved in neutron scattering research with easy access to beam time.

- Support of special European workshops and conferences with the aim to bring different communities in materials science and basic science together to exchange the potentials of neutron scattering-based research in materials science and development.

To make access to the facilities easier, particularly for non-specialized materials researchers, who do not want to get too much involved into the techniques, but just want to use them for their development purposes, special measures have to be taken at the neutron scattering centres themselves. Most centres are presently organized in a way to support only relatively experienced users, a situation that is not very helpful for the use of standardized methods of characterization with high throughput. In order to improve the situation for the non-industrial materials science community, the following measures are proposed:

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- Support of specific "Local contacts for materials characterization" of this community at relevant neutron scattering facilities, staffed with personnel (scientists, engineers) that are experienced both in the use of neutrons and in materials research. They should be the primary contacts for materials researchers from the different institutions in the European community.

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7.3. High-Resolution Microscopy

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Direct imaging of materials has always been an important aspect of microstructural characterization. There are various techniques for different wavelengths and instruments, namely, optical microscopy (wavelength in the range of that of visible light) scanning electron microscopy (SEM) and transmission electron microscopy (TEM) (wavelength in the Ångstrøm or sub-Ångstrøm range) [1]. While optical microscopy is a rather mature technique, SEM and TEM have undergone major developments and advancements over the past decade. These advances have been made possible by revolutionary progress in instrumentation. It is now feasible to correct fundamental aberrations of electron optical instruments. In addition, it is now possible to generate coherent electron sources. Improved detection systems exist which allow the detection of each electron. Furthermore, advancements in the understanding of elastic and inelastic scattering of high-energy electrons by crystalline and non-crystalline materials lead to a quantitative understanding of the collected data.

In this chapter only transmission electron microscopy will be considered. Other new and advancing imaging techniques will be covered in Chapters 7.4 and 7.5.

A major goal in materials science is the imaging of materials at the atomic level. This requires instrumentation allowing the theoretical and practical achievement of atomic resolution [2]. Resolution in the Ångstrøm range can be reached by systems which use coherent waves of a short wavelength and are equipped with imaging lenses with sufficiently small aberrations. Atomic resolution of the bulk material is so far mainly achieved by TEM. So far atomic resolution can either be reached by increasing the electron acceleration voltage (at constant aberration) or by specific techniques which allow to eliminate indirectly lens aberrations by complex procedures (Table 7.5 [3]). However, recent developments in instrumentation allow the correction of aberrations [4]. With the latter revolutionary development aberration-free imaging should be possible in the sub-Ångstrøm range.

Elastic and inelastic scattering of electrons occurs in a specimen irradiated with electrons. Both types of scattered electrons can be utilized for the structural and chemical analysis of the materials and can be obtained with high spatial resolution.

It is expected that a major breakthrough is within immediate reach regarding quantitative high-resolution transmission electron microscopy (QHRTEM) for the investigation of both the structure and composition of materials with very high spatial resolution.

7.3.1. State of the Art

Transmission electron microscopy has made outstanding contributions to materials science with respect to the characterization of the microstructure of materials [2]. This covers not only structural aspects but also aspects of the composition of materials. The study of the microstructure of crystal lattice defects and interfaces is essential for

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Methods	Advantages	Problems	Complexity	Cost
HVEM	Available now Interpretability Large space in lens gap Localization of electron beam	Radiation damage (?) Detectors	Maintenance Building	$10M + building + service contract + technician salaries
Focus Variation Technique	Convertibility	Increased Dose Processing time	C_s must be known to less than 1%	Full microscope package ~$1.5M
Off axis Holography	Convertibility	Limited specimen area (near thin edge)	Biprism fabrication & operation C_s must be known to less than 1%	Full microscope package ~$1.5M
STEM	UHV environment Microanalysis Direct interpretation	Contrast/dose rate		300 kV - $2M 100 kV - $1M
High field	Stability	Not available yet Needs new materials Restrictive geometries	Lens fabrication Cryogenics Operation	(Developmental Costs)
Micro Lenses	Size Cost Reflection Mode	Not available yet Restrictive geometries Penetration	Interpretation	(Developmental Costs)
C_s-Correctors	Flexibility	Imminent, but not yet available Absence of low frequencies	Needs FEG	High developmental costs (>$3M) otherwise incremental ($100k)
Point projection	Lensless	Interpretation Field sensitivity	Tips	Moderate ($100k)

Table 7.5. Different approaches for extending atomic resolution microscopy [3].

understanding the physics of structural as well as functional materials. Contributions by TEM have been made in semiconductor technology of electronic device materials, in high-temperature superconductivity as an example for functional materials, and the mechanical properties of grain boundary fracture and failure for structural materials (for either single phase materials or composite materials).

There exist different paths for high-resolution imaging (Fig. 7.6). Coherent illumination (Fig. 7.6a) of the specimen with a fixed beam results in coherent scattering of all atoms of the illuminated area of the transmitted specimen. The exit wave at the exit surface forms by interference of the coherently scattered electrons. The most critical lens for this system is the objective lens, which generates the first image of the imaging lens system of the microscope.

For incoherent illumination (Fig. 7.6b) a small probe (as small as possible) is formed by the illuminating systems.

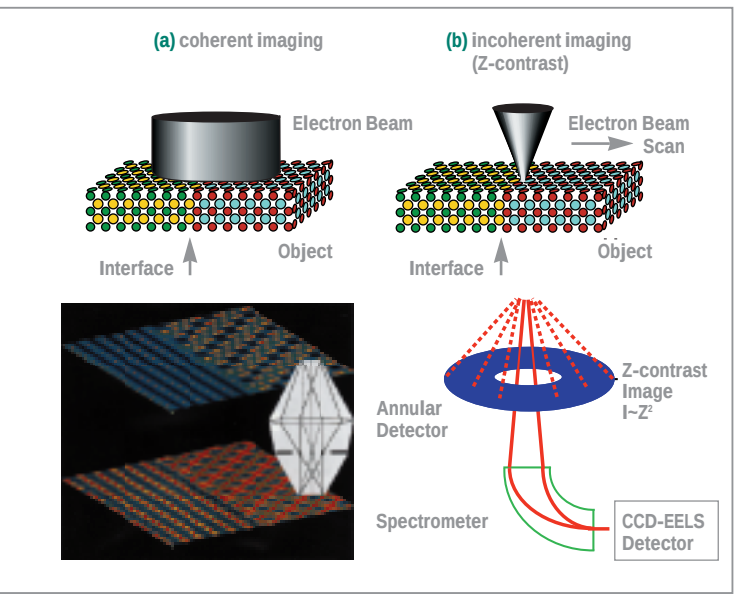

Fig. 7.6. Image formation in a high-resolution transmission electron microscope: **(a)** Coherent imaging (left column): The specimen is irradiated with a coherent electron beam (beam diameter larger than interatomic distance). At the lower foil surface the amplitudes and phase fields of the different scattered waves are formed. The aberration of the lenses modifies the wave field. The quality of the image depends strongly on the contrast transfer function [2]. **(b)** Incoherent imaging (right column). The specimen is transmitted with a strongly focussed electron beam (beam diameter smaller – if possible – than the interatomic distances). The beam is scanned over the specimen and the signals detected arriving at a large angle annular detector. The chemical analysis is performed by a spectrometer. Compared to coherent imaging the contrast transfer function is rather simple. The image interpretation for both imaging techniques is not trivial [2].

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The elastically scattered electrons are detected on a large-angle aperture. The probe is scanned over the specimen and the intensity of the scattered electrons is determined simultaneously. The most critical lens represents the probe forming system.

A very active demand for high-resolution electron microscopy (HRTEM) comes presently from the rapidly developing field of electro-ceramic materials where e.g. defect-related dielectric losses and the atomic perfection of internal interfaces are critical issues. The structure of grain boundaries in $SrTiO_3$ has been analysed by HRTEM, one example is shown in Fig. 7.7.

For structural and compositional investigations by TEM the quality of electron optics is limited so far by intrinsic aberrations of electro-magnetic fields forming the lenses for electrons. Although aberration corrected systems are standard in light optics since the beginning of 20th century, it is only recently that the feasibility of corrected electron optics could be demonstrated. In 1998 it was shown by a German research group [4] that the primary resolution of an ordinary commercial 200 kV TEM equipped with a field emission electron source can be almost doubled from 0.24 nm to 0.13 nm. The quality of the electron microscope images is significantly improved by compensation of the spherical aberration of the objective lens by means of an electro-magnetic hexapole lens system. Similarly, electron optical elements which correct spherical aberrations for the probe forming lenses in a scanning transmission electron microscope (STEM), reduce the diameter of the incoming beam of about 2 Å at the present to less than 1 Å in the very near future [5].

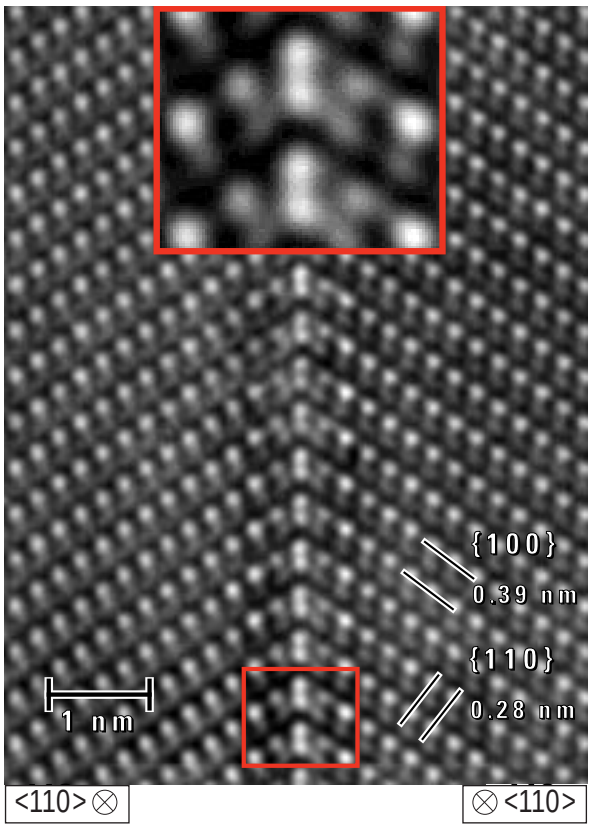

Fig. 7.7. HRTEM image of a highly symmetrical twin grain boundary in $SrTiO_3$ [Σ3 (111)]. Coherent image recorded in <110> projection. The inset at the top shows an enlargement of the framed region at the bottom. By quantitative evaluation of HRTEM images the positions of the atom (ion) columns near the grain boundary plane were determined with an average precision of 0.015 nm. (From Kienzle et al. phys. stat. sol. (a) 166 (1998) 57).

With respect to HRTEM imaging, impressive results could be obtained on the structure of (internal) grain boundaries and interfaces between dissimilar materials. The position of columns of atoms can be revealed with an accuracy of ≤ 0.3 Å depending on the nature of the composition of the corresponding columns. One example of the interface between Cu and α-Al_2O_3 is shown in Fig. 7.8.

Analytical electron microscopy (AEM) uses inelastically scattered electrons for the determination of the composition of small cylinders within the material. The diameter of the cylinders (beam diameter) ranges from about 0.5 nm to 1.0 nm in a dedicated STEM. The inelastically scattered electrons contain information on composition, coordination and bonding of atoms. The structure and chemical composition in such a cylinder (including the account of broadening of the electron beam due to scattering processes within the specimen) can be determined with high precision by electron energy loss spectroscopy (EELS). Energy loss near-edge structures (ELNES) reveal local features in the band structure of unoccupied states with high spatial resolution [2]. In principle, this can be also be obtained from regions at interfaces, dislocation cores and other structural defects. Information on bonding at those defects can be gained. So far, however, the beam diameter exceeds the interatomic distance at grain boundaries or interfaces. Therefore, contributions of the bulk material are included in the spectrum, making it very tedious to get information on bonding just from the area of the defect in the material.

It is expected that the bonding across defects can be extracted. However, sufficient spatial resolution and energy resolution is not yet attainable. This is also due to the low transmissivity and dispersion of the spectrometer. The present commercially available energy resolution of the dispersive component is in the order of 0.7 eV. Such a description does not allow the distinction of details of the spectrum since essential features are convoluted by the low energy resolution. Advanced instrumentation with an energy resolution in the order of 0.2 eV is required and will be obtained soon.

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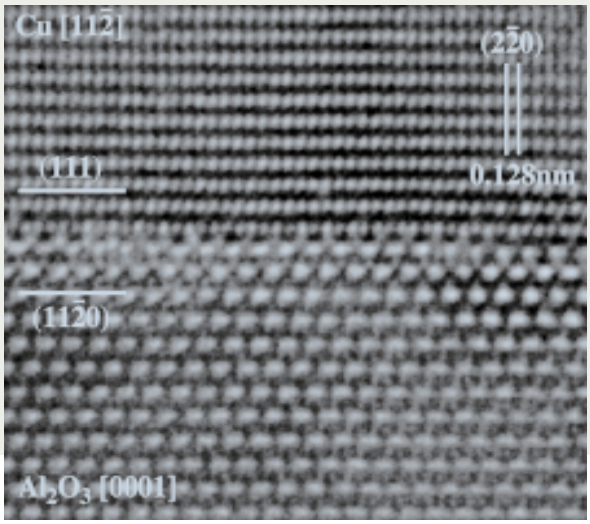

Fig. 7.8. HRTEM image of the atomically abrupt Cu/(11$\bar{2}$0)Al_2O_3interface taken along the [11$\bar{2}$]Cu zone axis. The HRTEM studies were performed on a JEOL JEM ARM 1250 microscope operated at 1250 kV with a point resolution of 0.12 nm. Image simulations assuming Cu-Al bonds at the interface as found by EELS studies exhibit a projected bonding distance of (0.15 +/- 0.02) nm to the first O-layer in the Al_2O_3 substrate. (From Scheu et al. phys. stat. sol. (b) 222 (2000) 199).

An important analysis technique is electron spectroscopic imaging (ESI) [6] where inelastically scattered electrons with a certain value of energy loss are used for imaging the specimen. This technique allows the element-specific determination of the distribution of different elements within a specimen. An energy loss is selected which is just beyond a characteristic absorption edge of the element in the energy loss spectrum. So far mainly qualitatively interesting results, especially for nanomaterials, could be successfully obtained.

A quantitative evaluation of HRTEM micrographs and analytical studies (especially by ELNES) requires the comparison of experimental observations with the results of simulations (Fig. 7.9). This is very important for HRTEM since the scattering process and image forming process within a specimen is highly non-linear, which often means that the position of strong contrast features does not coincide with the (projected) positions of atoms or columns of atoms. The determination of the reliability (error bars) is obtained by shifting the atoms in the model configuration and calculating the image again. Significant deviations between experimental intensity distributions and the newly formed model configuration result in the error bars.

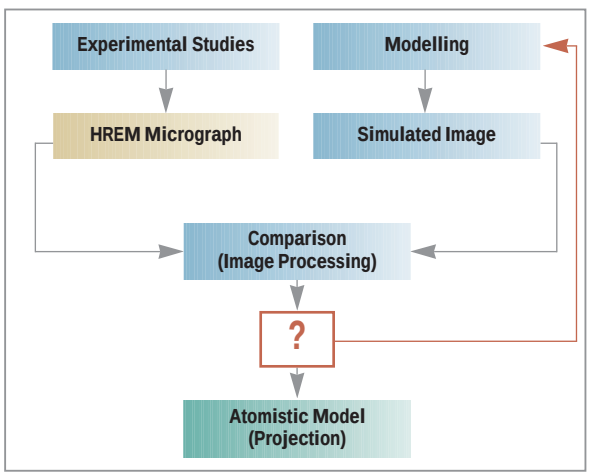

Fig. 7.9. Quantitative evaluation of HREM micrographs.

7.3.2. Future Visions for Transmission Electron Microscopy

Due to the availability of corrector elements for spherical aberrations there will be a revolutionary step for the further development of TEM with respect to atomic, structural and spectroscopic resolution. Advanced instruments presently under development will allow a spatial resolution in the 0.7 Å regime. Enormous efforts are being made to ensure the stability of an instrument so that no external disturbances (variations in high voltage and lens currents) and environmental effects (electromagnetic stray fields and mechanical vibrations) impair the theoretically achievable resolution of the instrument. In addition, high demands are imposed on ideal specimens since contamination and deviations of the atomic flatness of surfaces may result in fluctuations which disturb the wavelength. The delivery of such instruments for high-resolution imaging (200 kV with field emission gun) is scheduled for 2003 (SATEM project of the German Science Foundation).

In addition, the combination of TEM with EELS for local analysis of elements in compounds and ESI will be available with instruments having a spectroscopic energy resolution in the range of 0.2 eV and with a spot size in the order of ~2 Å. The prototype of the (so-called) SESAM (Sub-eVolt-Sub-Ångstrøm Microscope) instrument [7] will become operational in 2002. The combination of high local structural resolution in space with high spectroscopic resolution in energy will provide science and technology with direct access to the local electronic properties in atomic dimensions. The spectroscopic energy resolution in the range of 0.2 eV permits to distinguish between different electronic valence states and provides access to impurity states and bonding at interfaces which is relevant for both structural and functional materials. Preliminary results of spectroscopy at the nearly atomic level is shown in Fig. 7.10 which depicts the column-by-column spectroscopy of a grain boundary in $SrTiO_3$ doped with Mn [8]. However, for this experiment the approximate diameter of the electron probe was larger than the diameter of the projected columns of the materials.

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The advanced instruments have in-column energy filters with a high transmissivity allowing imaging modes in which solely electrons which have experienced a specific energy loss are used to form an image. Hence, element selective imaging is available. This provides the researcher with chemical maps of the investigated sample material which also possess high lateral resolution.

The art of *in situ* experimentation was widespread during the period of high-voltage electron microscopy in the seventies and eighties. In fact the pole-piece dimensions of a 1000 kV transmission electron microscope are intrinsically larger compared to those of a classical 200 kV instrument. By now *in situ* experimenting in high-voltage microscopes has essentially disappeared mainly due to the uncertain effects of the radiation damage introduced into the materials by high-energy electrons. It is to be expected that a new generation of dedicated, aberration corrected 200 kV instruments, which are much less expensive and fit into a normal laboratory room, will bring about a renaissance of *in situ* experimenting. Not only that a fairly high-

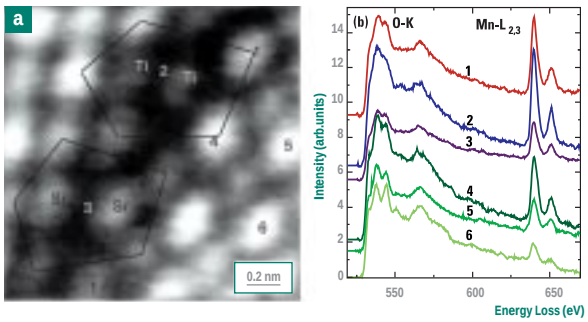

Fig. 7.10. (a) Z-contrast image of a Mn doped 36.7° <100> tilt grain boundary in $SrTiO_3$.The structural units, which are similar to dislocation cores, and locations of the probe where spectra were taken, are indicated. **(b)** The EELS spectra from the indicated locations after background subtraction show differences in the chemical content and the near edge structure from different atomic columns at the grain boundary. (From Duscher et al. phys. stat. sol. (a) 166 (1998) 327).

resolution is available for the *in situ* observations during specimen treatment, e.g. deformation, heating, cooling or while the specimen is in a controlled gas atmosphere or in an electronic function, the instrument's spectroscopic accessories will permit immediate analysis of the states traversed or of the products. In addition, the recent progress in micromachining and micromechanics, in particular on the basis of silicon, permits entirely novel micromanipulation devices. Hence, a new generation of dedicated aberration-corrected transmission electron microscopes optimized for *in situ* experiments will provide materials science and technology with fascinating new and unique possibilities for dynamic investigations in the nanometre- and sub-nanometre regimes.

Owing to the huge development costs the electron optics industry requires the backing provided by a sufficient number of orders to reduce the commercial risk to a manageable level. This requires supraregional procurement programmes. The stimulus for industry to develop the new technology for the benefit of all future potential users goes parallel with the early availability of the new instruments for those whose orders were placed early. The core components of aberration corrected microscopes and spectrometres are produced in rather small companies whose capacity is limited. Only a relatively small number of instruments can be manufactured at a time. Delivery times of the order of three years or more are realistic, simply due to limited manpower in development and fabrication. Therefore, an element of the international competition of users will be their respective position in the pipeline of orders. The first procurement programme funded by the German Science Foundation (Deutsche Forschungsgemeinschaft) together with the State of Baden-Württemberg, the Max-Planck-Society and the Helmholtz Research Centre at Jülich will lead to a first generation of commercial aberration corrected and high-precision spectroscopy instruments. The experience with these instruments will provide a solid basis for the funding and efficient operation of an improved second generation of instruments, to be purchased and disseminated in a European-wide framework.

7.3.3. Needs and Trends in Electron Microscopy Techniques

Recently, breakthroughs have been achieved in the microscopy techniques described in this chapter: The correction of lens aberration with advanced instruments leads to a marked improvement in resolution of all types of electron microscopy techniques. Furthermore, the possibility of generating small probes in the sub-Ångstrøm region allows the chemical analysis with atomic resolution.

It is expected that the improved instrumentation (Fig. 7.11) will lead to impressive new results in materials science. However, there is still the need for continued education in the area of electron optics and imaging techniques, an area that is slowly disappearing in Europe. Furthermore, the interpretation of the results obtained requires theoretical studies of the investigated systems. This will lead to an understanding of structure, composition and bonding on the atomic level.

New frontiers will be reached with the introduction of the next generation of TEMs. Expected results are summarized in Table 7.6.

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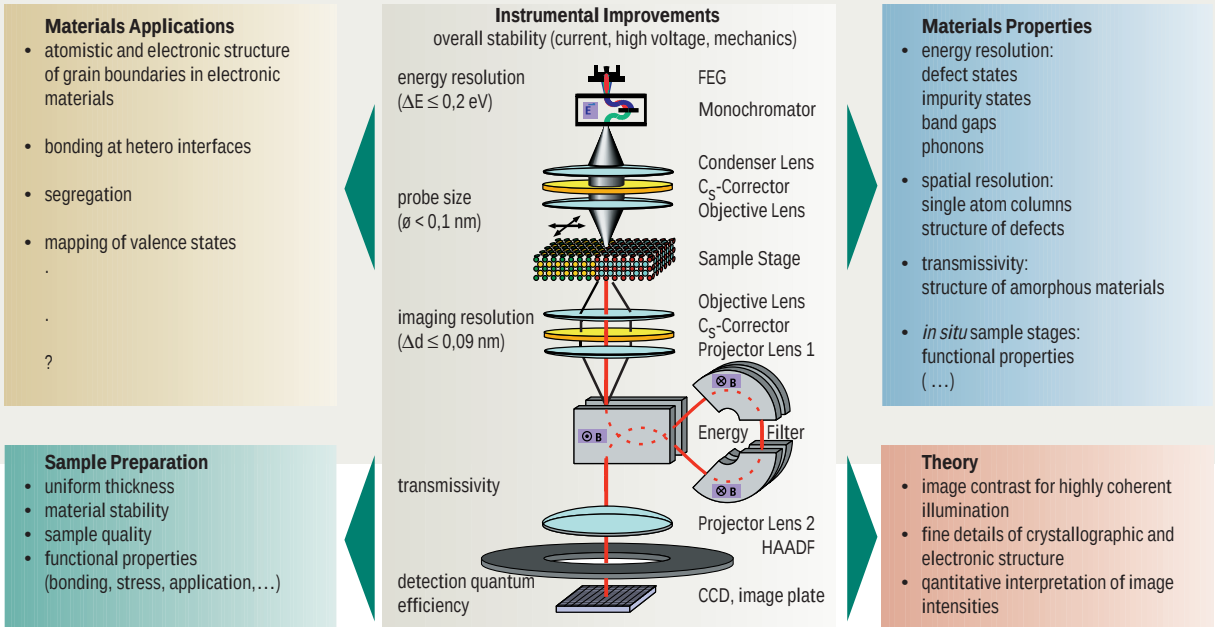

Fig. 7.11. Properties and Implications of the Future Transmission Electron Microscope.

Problems to be solved by Advanced TEM
Bond charge distribution in crystalline materials
Interface science
Defects by deformation and irradiation
Phase transformation and alloy design
Nanostructured materials
Surfaces and thin films
Microelectronic materials and devices
Structure of amorphous materials
Structure of confined amorphous materials

Table 7.6.

There are urgent measures to be taken by the EC within the 6th Framework Programme in order to support and coordinate the different activities in Europe and to link the different institutions together. It is also important that advancements made in different laboratories are made available to all interested research groups. It is also expected that research centres similarly to those for X-ray studies, are established where state-of-the-art instruments are operated.

In addition, theoretical investigations require the establishment of centres which are strongly collaborating with theoretical groups to compliment the experimental studies.

The following measures are proposed:

• Support of European interdisciplinary networks on transmission electron microscopy techniques in materials science. These networks should include all leading research groups in this area with a constant exchange of the latest advancements in instrumentation, interpretation and theoretical modelling.

• Application laboratories should be established that provide easy access to state-of-the-art techniques. The function of such laboratories would also be combine fundamental and applied research.

• There is a strong need for continued education in electron optical imaging. This field is rather mature. However, recent developments show that it is essential that the activities in theoretical optics will continue over the next decades. These chairs should be closely linked to transmission electron microscopy technique laboratories.

• Creation of special fellowships for doctoral students (e. g. Scherzer fellowships) which should be made especially available to students from countries who do not have advanced instruments at their students' disposal.

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7.4. Surface Science and Scanning Probe Microscopy

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7.4.1. Introduction with General Remarks on Surface Science Techniques

The investigation of material surfaces is an advanced area of study in solid state science and materials science. A variety of different imaging and diffraction techniques exist that allow the characterization of surfaces at the atomic level. The surface often serves as a platform to investigate fundamental aspects of materials science, such as crystal growth (e.g., epitaxy), chemical reactions (e.g., oxidation and corrosion), and catalysis. Surface science often acts as a "window" for investigating the microstructure of the bulk material.

A classical technique from the early days of materials science involves surface-level observation of glide steps by replica techniques. From these surface-level studies, models for the plastic deformation of the materials could be developed.

Instrumentation for the investigation of surfaces has become standard laboratory equipment. Optical microscopy and scanning electron microscopy (SEM) [1] are widely used techniques. Significant advancements in SEM instrumentation allow the observation of surfaces under very high-resolution in different gaseous environments of the specimen. It is now standard practice to use instruments with a field-emission source and specific electron optical lenses. Chemical information obtained with SEM can be analysed by energy-dispersive X-ray spectrometry (EDS) of the inelastically scattered electrons. The spatial resolution of this technique depends on the pear-shaped excitation volume of incoming electrons underneath the surface.

For an electron energy of ~30 keV under SEM observation, the diameter of this excitation "pear" is about 1 µm. A reduction in electron energy reduces this diameter; however, the X-ray yield is also reduced. Furthermore, the electron energy has to surpass the electron excitation energy threshold. Therefore, the excited volume of the specimen can only be modified in a very limited way by varying the energy of the incoming electrons.

Other surface-science techniques (see Table 7.7) include X-ray photon spectroscopy (XPS), Auger electron spectroscopy (AES), electron probe microanalysis (EPMA), and secondary ion mass spectroscopy (SIMS). Instrumentation of these various techniques is highly developed and improved. A major task has been the quantification of data, which also includes a correct description of error bars and reliability. These various classical surface science techniques are useful when studying specific qualities and constraints. XPS is mainly used to get information on the chemical state of atoms at the surface. Successful efforts have been made to improve their rather poor lateral resolution; the depth resolution is a few atomic layers. The strength of AES is its ability to measure chemical composition at the surface within a surface region of about 10 nm in diameter. Efforts are also being made to extract information about the chemical state of relaxing atoms from the shape and position of the AES signal. EPMA provides quite accurate quantitative local chemical composition (which also includes heavier elements with high-order numbers). However, the information stems from the pear-shaped volume of ~1 µm diameter underneath the surface. SIMS allows the detection of elements in a very small concentration, but the technique suffers mainly from an inaccurate quantification of higher concentrated elements.

In summary, the following instrumental research projects are currently under development: (1) reducing the information/response volume by increasing the spatial (lateral or vertical) resolution, (2) increasing the energy resolution in order to detect even small signal shifts or fine structures, (3) and decreasing the detection limit by increasing the signal-to-noise ratio. Furthermore, a layer-by-layer analysis would be preferable for the study of thin-surface films. Today, "depth profiling" by an ion-sputtering removal of surface layers can be performed with high reliability and high-depth resolution on the order of a monolayer. This technique, however, is limited by physical constraints [2].

Integrating different surface science techniques described above into one instrument is a promising goal.

Information on the relative orientations of crystalline grains in a polycrystalline material can be retrieved by means of electron back scattering diffraction (EBSD). EBSD can be used to investigate texture on very small scales [3].

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Requirements	XPS	AES	EPMA/WDS	SIMS	SEM/EDS
Quantification	+	o	++	—	o
Detection limit	o	o	+	++	o
Energy Resolution/ chemical shift	++	+	o		-
Mass resolution				++	
Image resolution	—	++	-	+	++
Lateral resolution	—	++	—	+	-
Vertical resolution	++	++	—	++	—
Depth profile	+	++	-	++	—

Table 7.7. Comparison of the different classical surface analysis techniques for determination of the chemical composition at the surface and in near surface regions (XPS: X-ray photoelectron Spectroscopy; AES: Auger electron spectroscopy, EPMA/WDS: Electron probe microanalysis using WDS (wavelength dispersive spectrometer); SIMS: Secondary Ion Mass Spectrometry; SEM/EDS: Scanning electron microscopy using EDS (energy dispersive spectrometer)). The classification is given depending on the possibility to fulfil the requirements: very good (++), good (+), medium (o), low (-) and very low (—).

In situ measurements made by different instruments result in dynamic studies of materials processes. Those investigations are extremely important for studying processes in catalysis, corrosion, and epitaxy.

A classical domain of *in situ* experiments in analytical electron microscopy (AEM) covers investigations of intergranular segregation on *in situ* intergranularly fractured surfaces, with one of the surface science instruments described above. Fundamental insight into the embrittlement process could be gained by this technique [4].

The classical techniques for the determination of surface-structure and surface-reconstruction results are diffraction studies of electrons of different energies: (1) low-energy electron diffraction (LEED), and (2) reflection of high-energy electron diffraction (RHEED). The back-scattered electrons are also being used to image surfaces (by LEEM and photo-emission induced electron microscopy, PEEM). The resolution of these images is on the order of 1 µm. Correction elements (see Chapter 7.3) have been included, allowing for the correction of aberrations, which results in a better image resolution. The latter experiments are now often being performed at high-brilliance synchrotron sources (see Chapter 7.1), resulting in high-intensity signals for better imaging.

All of the "classical" surface science studies discussed in this chapter were first performed during the mid-twentieth century, resulting in mature, user-friendly instrumentation. The instruments operate in an ultra high vacuum (UHV) and are quite costly. Typically, existing service centres in Europe make all surface science techniques available for interested materials science "customers." Materials science research would benefit from making these European centres linked and collaborative.

Binnig, Rohrer, and Gerber [5] invented in 1982 the scanning tunnelling microscope (STM). This invention revolutionized and advanced the fields of surface science. In the same year they observed tunnelling through a controlled vacuum gap and imaged single atom steps. In 1983 silicon (111)-(7x7) reconstruction was imaged in real space for the first time, marking the birth of a new field [6]. A decade later, STM gained worldwide use.

Shortly after the invention of the STM the atomic force microscope (AFM) was in operation. With this instrument also non-conducting materials can be investigated. Other techniques were developed when the probe (often an atomically sharp tip) is scanned over the surface of the material. Different interactions between tip (probe) and surface can be utilized for the measurements of different interactions (mechanical, magnetic, electric) under different atmospheres. All scanning techniques are subsumed under the expression of scanning probe microscopy (SPM).

The development of a specific scanning probe microscope (SPM) is essentially a method for making localized measurements of any property for which a detection scheme can be devised. Detection strategies are now available for probing first order, second order, and third order response functions to interactions. Thus it is now possible to detect, e.g. thermal gradients, magnetic forces, photon emission, photon absorption, piezoelectric strain, electrostriction, magnetostriction and optical reflection with localized probes. The remainder of this Chapter will deal with SPM. This technique is having a major impact in materials science, specifically in nanotechnology.

Scanning tunnelling microscopy, scanning probe microscopy, and atomic force microscopy, in general, have had a dramatic impact in fields as diverse as materials science, semiconductor physics, biology, electrochemistry, tribology, biochemistry, surface thermodynamics, organic chemistry, catalysis, micromechanics, and medical implants. The reason for the nearly instantaneous acceptance of SPM is that it provides three-dimensional real-space images of surfaces at high spatial resolution. Images are based on different signals detecting the local interaction between a small probe tip and the investigated surface. Depending on the particular SPM, the image can represent physical surface topography, electronic structure, electric or magnetic fields, or any other local property. SPM allows imaging at unprecedented levels of resolution in different materials, even organic tissues and large organic molecules, without damaging the samples. This is in contrast to other microscopy techniques, including SEM and transmission electron microscopy (TEM).

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7.4.2. State of the Art

In this section STM will be predominantly considered, similar results and rules can also be considered for other SPM techniques.

In the early stages of STM there was no clear understanding of the detailed mechanism underlying the contrast formation. Recent developments published in original publications or several textbooks reveal the principles of electron tunnelling between a real tip and a real surface. The theory is presently well developed and comparisons between theoretical calculations and experimental observations result in reasonable agreement.

A description of the state of the art is most likely obsolete by the time a book or report is written. There are a number of reasons for this. Experimental conditions are always improving. The capability to determine the atomistic structure can be done quite easily online, using very simple and inexpensive equipment (compared to big diffraction and imaging microscopes). However, an understanding of the basic principles of image formation by tunnelling processes as well as by atomic force interactions has recently been revealed [6,7]. Therefore, a discussion of the state of the art in light of these newly revealed principles is relevant.

Data analysis of topography and spectroscopy images of which I-V curves for a fixed probe position can often be determined and detected is rather straightforward. Comparisons of microscopy data to scanning tunnelling spectroscopy (STS) calculations showthat there is good agreement between experiments and theory. Details of the spectroscopy are widely understood. This also includes the electronic structure of the tip and tip-induced bending of Fermi surfaces.

Spectroscopy leads also to the investigation of inelastic tunnelling spectroscopy of, for instance, energy barrier heights at interfaces. The unique ability of STM to probe the electronic structure of surfaces directly has opened another dimension in our understanding of surfaces by allowing the study of electronic states at the surface on an atom-by-atom basis. STM directly correlates the geometric positions of atoms with their resulting electronic structure.

STM investigations of surface structures and of structural or compositional defects at surfaces opened a completely new and unexpected dimension of materials science. While diffraction studies by LEED usually are obtained from a large area, individual defects and defect agglomerates can be investigated by STM at surfaces and these studies lead to an understanding of critical properties of surfaces and reactions at surfaces (Fig. 7.12).

The STM technique is also applied to investigations of crystal growth. For instance, studies of the growth of metals on different conducting or non-conducting ceramics have led to a much better understanding of nucleation and growth of metallic films on different substrates.

The imaging of the electrostatic potential leads to an understanding of domains in electronic and magnetic materials. Although, the interpretation of the images is not easy, it gives deep insight into the magnetic and electronic structure of surfaces. Often also information with respect to grain boundaries in the crystals can be gained.

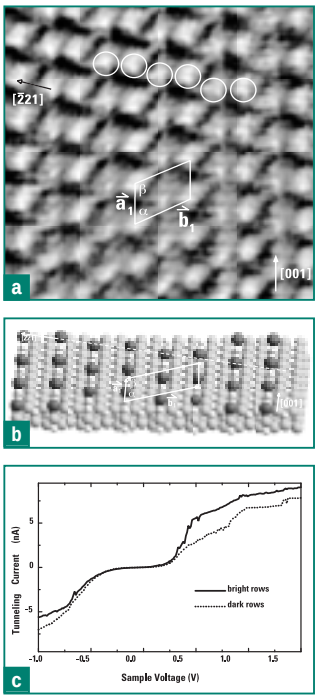

Fig. 7.12. (a) High-resolution STM image of an atomically flat terrace of the TiO_2 (110) surface obtained in constant current mode (V_{bias} = 1.67 V, I_t = 0.6 nA), with a black-to-white scaling of 3 Å. The unit cell of the reconstruction is displayed. **(b)** A plane view of the proposed model for the reconstructed TiO_2 (110) surface. Large dark spheres represent O-ions in the bridging oxygen rows, large gray spheres are due to in-plane O-ions, and small black spheres represent Ti^{4+}. The dimensions of the unit cell are a_1 = 8.85 Å and b_1 = 14.26 Å, and the angles are α = 65.5° and β = 114.5°. **(c)** Scanning tunnel spectra from the TiO_2(110) surface acquired from bright and dark contrast regions in the image. (Wagner et al. Appl. Phys. A 66 suppl. (1998) 1165).

An understanding of microelectronic devices requires the understanding of the physics of the carrier transport through thin films and across interfaces. These investigations have been successfully performed by ballistic electron emission microscopy (BEEM). This STM technique comprises a family of spectroscopies that addresses the transport and scattering of electrons and holes in multilayered structures. Successful results, especially with STM surpass all experimental results obtained so far by other surface science techniques.

AFM can be applied to the study of topography and interactions between the tip and the surface of a conducting or nonconducting material. Enormous progress has been made for different structures, especially functional materials from which information about electronic, electric, and magnetic properties can be obtained. Furthermore, AFM can also be applied to liquids and organic specimens, leading to an understanding of processes in a cell's DNA on the nanometre scale.

Furthermore, AFM techniques can be used for nanomechanics investigations. For such studies, the tip of the AFM is used for two aspects: (1) the tip of the AFM is employed to produce indents in a specimen, and (2) friction measurements can be done by scratching the tip over a surface. The mechanical forces are then measured with a special attachment to the AFM. Information on the materials can be obtained on a nanometre scale. The modification of the surface by the test can then be made visible by imaging the surface after the test in an imaging mode.

7.4.3. Future Perspectives

It is quite obvious that SPM techniques are instrumental in the investigation of processes in the nanotechnology world. AFM is an adequate technique to investigate surface topography, small particles and modifications of those through different treatments. However, an enormous impact can be expected by combining the different measurement techniques (e.g. magnetization or electrical forces) with properties sensitive to topography. One promising technique includes also the combination of SPM and near field scanning optical microscopy (NSOM). With the latter technique the diffraction-limited resolution of optical microscopes can be overcome. The combination of the different techniques will definitely have an interesting impact on high-resolution imaging of solid and soft surfaces of materials.

The different SPM techniques can be applied to get information on bulk materials by investigating defects close to surfaces which are, of course, connected to the underlying bulk. The application to soft materials will allow the successful investigation of single molecules extending the field to nonperiodic materials.

The great advantage of all SPM techniques is the ability to do time-resolved investigations which give an insight into atomic or near-atomic processes in all materials.

One exciting challenge for the improvement of SPM will be the development of sensors than can produce valuable quantitative results. For example with the availability of very sensitive force transducers in the range of nN (e.g. mechanic, friction, magnetic or electric) forces can be measured and also applied to investigate the local response of the materials. This will be a springboard for the understanding of fundamental phenomena like adhesion, surface reactions, friction, tribology, wetting. The ability to manipulate materials at the atomic scale will be an impetus for next-generation research in the broad field of nanotechnology.

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7.5. Three-Dimensional Atom Probe

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7.5.1. Introduction

Atom probe microscopy was first performed in 1951 by E.W. Müller at The Pennsylvania State University when he imaged individual atoms with a field ion microscope [1]. His very impressive results show the structure of the surface of a tip of tungsten where each bright spot corresponds to a single atom. Since that time, enormous progress has been made in instrumentation, especially in signal detection and processing. The most recent advance is the 3-D atom probe technique (3DAP), which is now firmly established.

The 3DAP traces its origin back to the field electron microscope. However, a number of steps had to be accomplished before the development of the 3DAP could occur. The atom probe microscope is based on the principle that electron emission from a solid can occur in the presence of a strong electric field. This technique was used to image surfaces; however, Müller introduced a new type of microscope in which the specimen was in the form of a sharp needle. Extremely high fields were applied, and with a large distance from the tip of the needle to a screen, high magnification of the simple imaging system was achieved so that atomic resolution images of the tip could be obtained on the screen. The next step was the introduction of an atom probe as a field ion microscope. This allowed, by time-of-flight analysis, investigation of the specific atom or sample region with a mass spectrometer. The fluorescence screen, which made the image visible, had a hole in its centre where the atoms coming from a selected region were analysed. The specimen (tip) could be adjusted by tilting the imaging screen.

Next was the introduction of an imaging atom probe, which meant that the number of atoms analysed from the specimen had to be increased by several orders of magnitude. This required the elimination of the channel blades and the screen assembly that contained the probe aperture that permitted the single atom detection to be positioned closer to the specimen. All atoms emitted from the specimen had to be detected simultaneously.

7.5.2. State of the Art

The present state of the art was achieved by the introduction of the 3DAP, originally developed by Blavette et al. [2] and Miller et al. [3]. The 3DAP is a position-sensitive atom probe that allows an atom-by-atom analysis at several different locations simultaneously over an entire screen. A fully operational system was first developed by Cerezo et al. [4]. The instrument features a single atom detector based on a pair of microchannel plates and a wedge and strip, or back anode. The X and Y coordinates of the ions' impact on the detector are determined from the relative charge measured on the free anodes in the wedge and strip detector. Additional details of the position sensitive atom probe can be found in the literature.

Continuous stripping of the specimen (layer by layer) in an automated way allows the determination of the atomic distribution of the different species through a thin cylindrical specimen in the microscope. Individual atoms can be detected and the atomic position can be determined with high accuracy.

This instrument allows the analysis of cylindrical parts of a specimen (with a diameter of about 30 nm and a length of about 200 nm), probing atom by atom through the specimen. The technique has enormous potential for the understanding of fundamental aspects of materials science, including segregation at grain boundaries, processes of nucleation in materials, radiation-induced defects, and decomposition of materials. Impressive results were also obtained on the thermal stability and interdiffusion in thin films.

An example of the ultrafine-scale information available with the 3DAP technique is shown in Fig. 7.13, which represents the atomic imaging of an Ω-phase precipitate formed in an Al alloy. Segregation to the surface of the precipitate can easily be recognized. The example illustrates the detailed, ultrahigh-resolution chemical information that is available with an advanced 3DAP.

Early 3DAP instruments suffered from a modest mass resolution. This was caused by the energy variations resulting when ions are accelerated during a voltage pulse. The problem was solved by Cerezo et al. by incorporating a large-acceptance-angle reflection lens into the instrument. this is presently the state of the art. The quantitative analysis of a specific stainless steel (see [4]) revealed e. g. the peaks of Ni, Cu and Mo can be clearly separated despite these elements being present at levels of less than 0.1 % and, in some cases, separated by only one-sixth of a mass unit.

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Impressive results could also be obtained for the studies of grain boundary segregation, although the specimen preparation is tedious and time consuming. A 3DAP analysis of grain boundaries in an "interstitial-free" (IF) steel containing 7 wt.% ppm of B revealed that B and C segregate at the grain boundaries with a Gibbsian interfacial excess concentration of 0.57 atoms/nm^2. It is quite remarkable that the segregation of B is not confined to a single atomic layer but is spread over a layer (parallel to the grain boundary) of about 1 nm thickness.

Similarly, solid state reactions and intermixing in technologically important thin layer systems could be analysed by the determination of the position and nature of individual atoms [5].

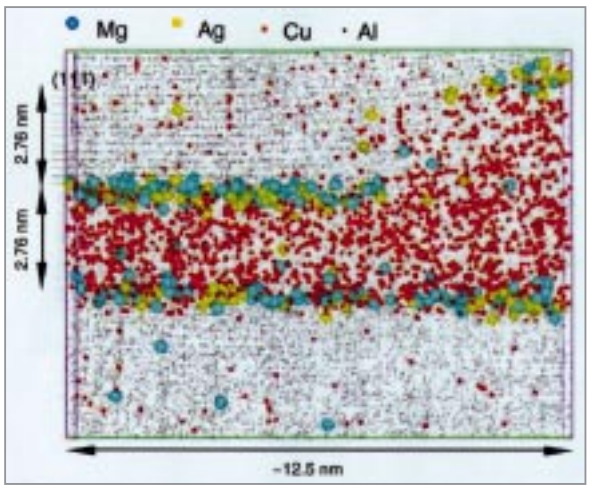

Fig. 7.13. 3DAP elemental map showing a step at the interface of an W phase precipitate formed in an Al-1.9 wt%Cu-0.3wt%Mg-0.2wt%Ag alloy aged at 180 °C for 10 h. Segregation of Mg and Ag to the precipitate interface is clearly observed, as is the enhancement of Cu in the vicinity of the step. (Courtesy H. Hono, National Research Institute for Metals, and Acta Materialia).

7.5.3. Future Aspects

Work on thin-film materials and devices will be further enhanced by current instrument developments to allow the use of specimens in the form of microtips fabricated on the surface of a planar substrate [5]. The basic principle behind such instrumentation is the use of scanning probe microscopy with the local electron atom probe. Microtip specimens are fabricated from thin films or devices on a planar substrate, either by masking and ion-beam milling or by the use of focussed ion beam (FIB) milling. Many hundreds of microtips could be made within a few mm^2, all with the layers of interest at the apex. However, advanced instrumental developments are required for such fabrication [5].

Results from the 3DAP still fall short of full atomic resolution (with high spatial accuracy), due to the presence of small trajectory aberrations that reduce the lateral resolution. The reason for this is poorly understood. Theoretical work has directed in several directions for the solution to this problem. If those aberrations were understood and corrected, the 3DAP would be an ideal instrument for structural and chemical analysis of real materials. Of course, a correlation of calculated structures (by computer modelling) with experimental results would also be important.

The leading research groups in the area of 3DAP are in Europe (Oxford, Gothenborg, Göttingen, Paris). To solve these 3DAP resolution problems, it is essential that these groups form a closely linked network.

Advanced 3DAP allows the measurement of individual atoms in the specimen volume, but also can detect small amounts of doped or contaminant elements. This is crucial for the understanding of their influence on desired and sometimes not desired macroscopic properties, for example, in microelectronic devices. With the availability of quantitative information on the number of atoms from each atom species and the place they occupy, it will become possible to reconstruct, for example, segregation or diffusion profiles in order to determine the respective rates and to understand via the "growth" laws the dominant processes. In principle, the separation of thermodynamic effects from kinetic ones is now a realistic prospect.

In the 21st century, the combination of the 3DAP with TEM and atomistic modelling may provide a springboard for the systematic development of the next generation of alloys and metallic multilayer devices. Atomic engineering of these materials is now a realistic prospect.

Furthermore, the combination of scanning probe microscopy (SPM) and atom probe microscopy may allow detailed manipulation of atoms. Individual atoms can be picked up by the SPM tip from a surface. The atom can then by analysed by atom probe microscopy. This technique may be the key to overcome the current limitations of the 3DAP concerning sample preparation, the restriction to conducting materials and to low sampling temperature.

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7.6. Laser Spectroscopy

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7.6.1. Introduction

Understanding the relationship between structure and function represents a central issue of basic materials research. Fundamental physical, chemical and/or biological properties and functions of materials are determined by the dynamics of elementary excitations in the ultrafast time domain, i.e. between 1 fs (1 femtosecond = 10^{-15} s) and approximately 1 ps (1 picosecond = 10^{-12} s). Such nonequilibrium and relaxation dynamics which are determined by microscopic interaction processes, can be observed in real-time by optical techniques using femtosecond laser pulses for inducing and probing the linear or nonlinear material response. Experiments with fs time resolution have provided a wealth of new information on transient electronic and vibrational properties of materials and on fast processes which are essential for realizing new functional properties [1].

The comparably high peak intensities of ultrashort optical pulses at moderate average power are essential for a quantitative characterization of the nonlinear optical properties of materials which are applied for optical frequency conversion, multiplexing and switching, processes underlying modern optoelectronic and all-optical information technology. With increasing data transmission and processing rates, optical information technology moves towards the ultrahort time domain, requiring the implementation of ultrafast technology into communication systems. This is illustrated in Fig. 7.14 showing different optical technologies and their characteristic time/frequency range.

The rapidly increasing relevance of nanostructured materials for research and technology calls for new techniques to optically address and analyze individual nanostructures and to transmit information between them. This has led to the development of new nanooptical techniques, in particular microscopies with sub-wavelength spatial resolution, which allow optical studies of single nanostructures [2]. The spatio-temporal dynamics of elementary excitations on a nanometre scale is accessible by combining nanooptical and ultrafast techniques.

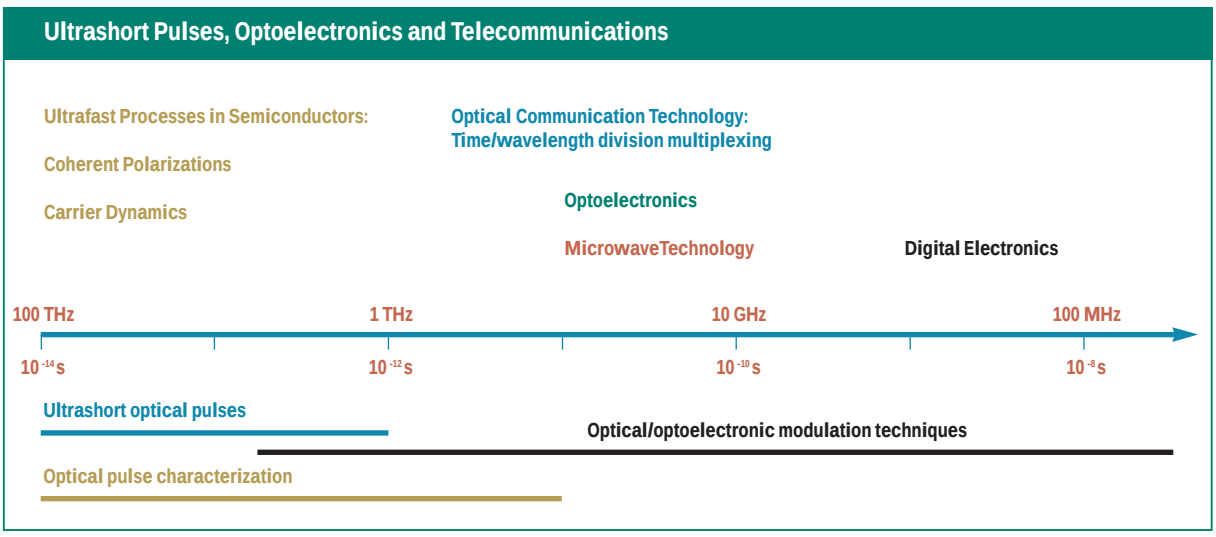
7.6.2. State of the Art

In this section, the state of the art of ultrafast material science and nanooptics is reviewed briefly and some future trends are outlined.

(a) Pulse generation, shaping, and characterization

Generation, shaping and characterization of fs pulses provide the basis for studying ultrafast processes and developing ultrafast technologies. Present technology is

Fig. 7.14. Characteristic time and frequency scales of optical and electronic technologies (upper part). In the lower part, the time ranges covered by ultrashort pulses, modulation techniques and optical pulse characterization are given.



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mainly based on mode-locked solid state lasers and amplifiers which are combined with nonlinear optical techniques for frequency conversion and with pulse compression methods. The wavelength range from 100 nm in the deep ultraviolet up to 300 µm in the far-infrared is now covered continuously with pulse durations of less than 200 fs. In addition, soft X-ray pulses at wavelengths between 5 and 100 nm and incoherent hard X-ray transients with wavelengths below 1 nm are available. The average output powers range from several µW up to about 10 W, the corresponding peak intensities are between several 10^3 W/cm^2 and 10^{15} W/cm^2.

Coherent pulse shaping techniques allow the generation of individual pulses or pulse sequences with tailored optical phase characteristics and the compression of pulses down to about 2 fs duration. For a phase-resolved characterization of pulses, methods like frequency-resolved optical gating, spectral phase interferometry, and electrooptic sampling are available. Highly sensitive techniques of nonlinear time-resolved spectroscopy are applied to monitor the ultrafast time evolution of optical polarizations and nonequilibrium populations.

(b) Ultrafast structural characterization

Ultrafast techniques which are able to grasp transient structures and nuclear motions in solids, liquids, and macromolecular systems play an increasingly important role for understanding microscopic transformation processes and chemical properties of materials. Temporally and spectrally resolved infrared methods are applied to monitor the creation, disappearance and the mutual coupling of functional groups in molecules through their vibrational absorption bands and to follow nuclear motions in real-time. Spectroscopic techniques of nuclear magnetic resonance (NMR) which works on substantially slower time scales, are being adapted for infrared spectroscopy in the pico- and femtosecond domain. First experiments have demonstrated the potential of two-dimensional infrared spectroscopy for structural characterization of biologically relevant molecules [3]. Time resolved X-ray diffraction represents another new, yet not fully implemented approach to study transient species, e.g. during phase transitions in solids or solid-liquid phase transitions [4].

(c) Imaging, microscopy and nanooptics

Ultrafast imaging methods, optical microscopy using femtosecond pulses, and nanooptical techniques provide direct information on the stationary and transient structure of materials. In optical coherence tomography (OCT), partly transparent biological materials, e.g. tissue, are irradiated with fs pulses and information on the spatial structure of the layer investigated is extracted from the time structure of the back-scattered light. This technique enables *in situ* imaging of the microstructure of materials and has found medical application. In multi-photon microscopy, fs lasers serve as a light source for multiphoton excitation of organic chromophores embedded in the samples. Two-photon microscopy has developed into a standard technique of biomedical imaging.

Imaging in the mid- and far-infrared (THz) range has become a tool for studying the structure of porous material and detecting specific material constituents, e.g. water traces. Here, fs optical pulses serve for the generation and phase-resolved detection of electric field transients in the THz range.

Microscopy with subwavelength spatial resolution, i.e. confocal and near-field scanning optical microscopy (NSOM), is applied for optical characterization of structures on a length scale of typically 50 to 100 nm. Though this spatial resolution is usually not sufficient to optically image nanostructures, single nanostructures can be addressed optically and local excitations can be created at a well-defined nanometre distance from a nanostructure. The electronic structure of individual semiconductor and metal nanostructures and single macromolecules as well as local disorder potentials in extended quantum structures like semiconductor quantum wells have been studied, partly at cryogenic temperatures. While those experiments provide information on stationary properties, confocal microscopy and NSOM with femtosecond pulses can map the spatio-temporal dynamics of material excitations. Such time-resolved techniques have been implemented recently and first experiments on carrier transport in low-dimensional semiconductor nanostructures have been performed. Near-field techniques have also been used to write nanometre structures onto materials.

(d) Areas of application

The techniques outlined above have been applied in the following areas of materials research:

- Bulk and nanostructured semiconductors: Coherent polarizations and their influence on the optical spectra, ultrafast redistribution and thermalization of nonequilibrium carriers, and carrier cooling and trapping have been studied in great detail. A closed picture of the hierarchy of relaxation processes has been established by combining experimental and theoretical research. Detailed knowledge exists on microscopic quantum coherence, Coulomb and phonon scattering, and on manybody and nonlinear optical effects. Coherent all-optical control has been demonstrated with excitonic polarizations and photoinduced currents. This research

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has led to semiconductor devices with completely new and/or strongly improved functional properties.

- Metals, metallic nanoparticles, and correlated materials including high-T_C superconductors: Single-particle and collective excitations of the carrier system, lifetimes of image states at surfaces and the related nonlinear optical properties including Faraday rotation and other magnetic phenomena, are being studied in experiments with sub-10 fs time resolution. Correlated materials represent a new field of research in which the investigation of low-energy excitations, e.g. close to or below the superconducting energy gaps, is particularly important, as the electronic structure and optical spectra at higher photon energies are not fully understood. In general, our knowledge in this field is still much more limited than for semiconductors.

- Phase transitions of solids and material processing with femtosecond pulses: Order-disorder phase transitions, e.g. melting, and optically induced changes of crystal structure are being monitored via changes of the nonlinear optical properties, e.g. through second harmonic generation at surfaces, and by detecting transient structures by time-resolved X-ray diffraction. Material processing and structuring with femtosecond pulses frequently occurs under nonthermal conditions and with reduced thermal load on the material, leading to an improved quality of the processed samples.

- Molecular systems in the liquid and solid phase, adsorbates on solid surfaces: The dynamics of electronic, vibronic and vibrational excitations as well as photochemical reactions are the main research topics in this field which is frequently called "femtochemistry". As chemical reactions involve nuclear motions on a 10 to several 100 fs time scale, ultrafast techniques are an ideal tool to follow the pathway of a reaction, identify transition states and monitor the formation of products. There are first experiments in which the outcome of a reaction has been manipulated by tailored pulses or pulse sequences, demonstrating the potential for optical control of chemical reactivity.

During the last decade, the number of research groups performing basic research on ultrafast phenomena has increased substantially. In Europe, there are now approximately 50 groups active in ultrafast material science, the main competitors being laboratories in the U.S. and – to somewhat lesser extent – in Japan. European scientists have introduced key innovations in ultrafast laser technology and are among the top researchers in several areas of basic research, e.g. solid state physics or ultrafast processes in soft matter. In Japan, a 10-years-programme on "Femtosecond Technology" aims at a combination of fundamental research with technological applications, mainly in telecommunications and ultrafast optoelectronics. Japanese groups play a leading role in optical telecommunications with ultrahigh data transmission rates. In contrast to Japan and the U.S., the interest and involvement of European industry in ultrafast material science is still very limited.

Ultrashort pulses

Pulse durations:	2 fs ($2 \cdot 10^{-15}$ s) - 5 ps
Wavelength range:	100 nm - 300 µm + soft/hard X-ray
Peak power:	up to 1020 W/cm^2

- Control and quantitative analysis of optical phase (electric field).
- Different measurement techniques for real-time probing of optical polarizations and nonlinear material excitations in the wavelength range indicated above. Time resolution up to about 5 fs.
- Control of material excitations by interaction with tailored pulses and/or pulse sequences.
- Nonthermal material processing with ultrashort pulses.

Nanooptics – optics on a sub-wavelength length scale

Near-field scanning optical microscopy (NSOM):	
Spatial resolution	> 20 nm (λ/20)
Temperature range	5 - 300 K
Detection sensitivity	single photons
Confocal microscopy:	
Spatial resolution	>250 nm (λ/2)
Temperature range	5 - 300 K (resolution >500 nm)
For both:	
Spectral resolution	determined by laser source and detection system
Time resolution	determined by laser source (> 50 fs)

Table 7.8. Summary of Experimental Techniques in Laser Spectroscopy.

7.6.3. Expectations and Needs

In the following, some future trends of research in ultrafast optics and nanooptics are outlined together with a crude estimate of the period after which major goals may be achieved:

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- New femtosecond sources: Compact low-cost fs sources pumped by semiconductor diode lasers and mode-locked lasers working at high (GHz) repetition rates for technological applications (including telecommunications). Sources for ultrashort hard (keV) X-ray pulses at kHz repetition rate for time-resolved X-ray diffraction and absorption. Development of new laser materials and components, e.g. high-power diode lasers for new pumping wavelengths. Phase shaping and nonlinear conversion of pulses in an extended wavelength range (2 to 5 years).

- New and much more sensitive techniques for investigating transient structures and phase transitions by ultrafast infrared and X-ray techniques represents a very important direction of research which could lead to revolutionary new insight into the properties of condensed matter. Both laser-based methods and the use of free electron lasers providing short hard X-ray pulses will be important (5 to 10 years).

- Optical coherence tomography with extremely short pulses (improved depth resolution) and in extended wavelength ranges (mapping of different constituents, 2 to 5 years).

- Mid- and far-infrared near-field imaging with sub-100 nm spatial resolution, single pulse imaging (instead of scanning methods). New local probe designs for sub-wavelength optical microscopy with improved spatial resolution including single molecule probes, higher sensitivity and stability of local probe microscopies, multi-probe microscopies (5 to 10 years).

An interdisciplinary research environment is essential for competitive and successful research on and development of new optical techniques. This requires a long-term combination of material science, engineering, physics, chemistry and biology in joint European projects and networks.

A rapid transfer of new techniques into materials research requires a close cooperation of groups developing techniques with those applying them as the feedback of users is necessary for optimizing new techniques.

Support of dedicated competence centers which provide experimental facilities for cooperative research and accept guest scientists also for longer periods, is recommended, as ultrafast experiments require expensive equipment and highly specialized knowledge and skills.

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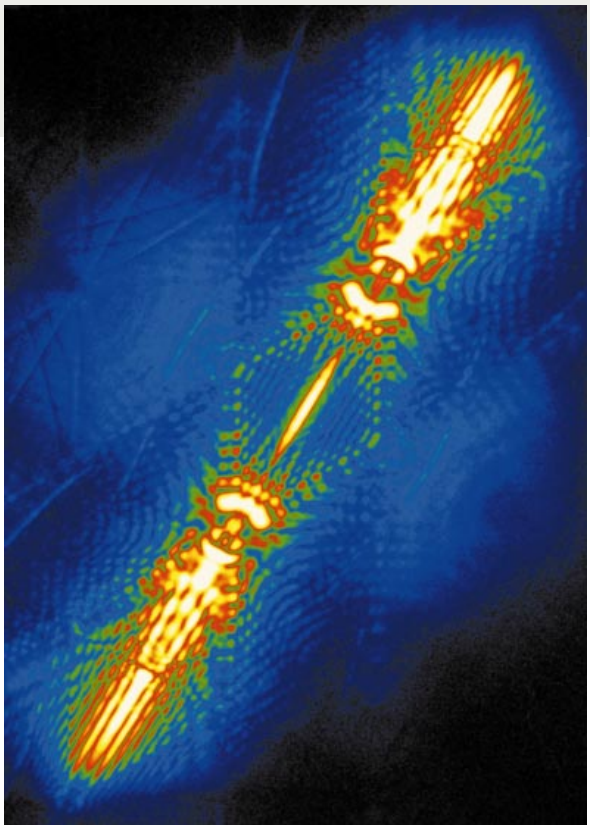

Convergent beam electron diffraction (CBED) pattern of Si. Details of (220) diffraction disc near the [III] zone axis. Information can be gained on the local bonding of atoms (ions) in the unit cell from the intensity distribution.

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7.7. NMR Spectroscopy

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7.7.1. Introduction

Precise knowledge of structure and dynamics of advanced materials is key to taylor them for specific functions. As an example, such diverse technological challenges as efficient fuel cells, photonic sensors & devices or gene delivery systems all require transport of electronics, holes, protons or other ions. This transport critically depends on the arrangement of the building blocks of the material relative to each other and their mobility on different length- and time scales. Even more informative for establishing structure/function relationships is the direct observation of functional carriers themselves. Solid state NMR spectroscopy has the potential of becoming one of the key methods to provide this vital information. In order to achieve this goal, however, a large scale effort on a European scale is required.

7.7.2. State of the Art

NMR Spectroscopy is one of the most powerful techniques for structural investigations. Sofar most applications focused on molecules dissolved in liquids, where NMR is an indispensable tool for the synthetic chemist, materials chemist or structural biologist alike. This was recognized by awarding the 1991 Nobel prize in chemistry to Richard Ernst, Zürich, for his eminent contributions to the advancement of this technique. New materials for future technologies, however, often function in the solid state, as highly viscous systems such as gels, or as molecules attached to surfaces. Moreover, such materials typically lack crystalline order in the traditional sense. Therefore, their structure cannot be determined with the required accuracy by the most established methods for structural elucidation, namely X-ray and neutron scattering. Here, solid state NMR provides the most promising approach Fig.7.15. Recent advances combining fast magic angle spinning (MAS), two-dimensional double-quantum NMR

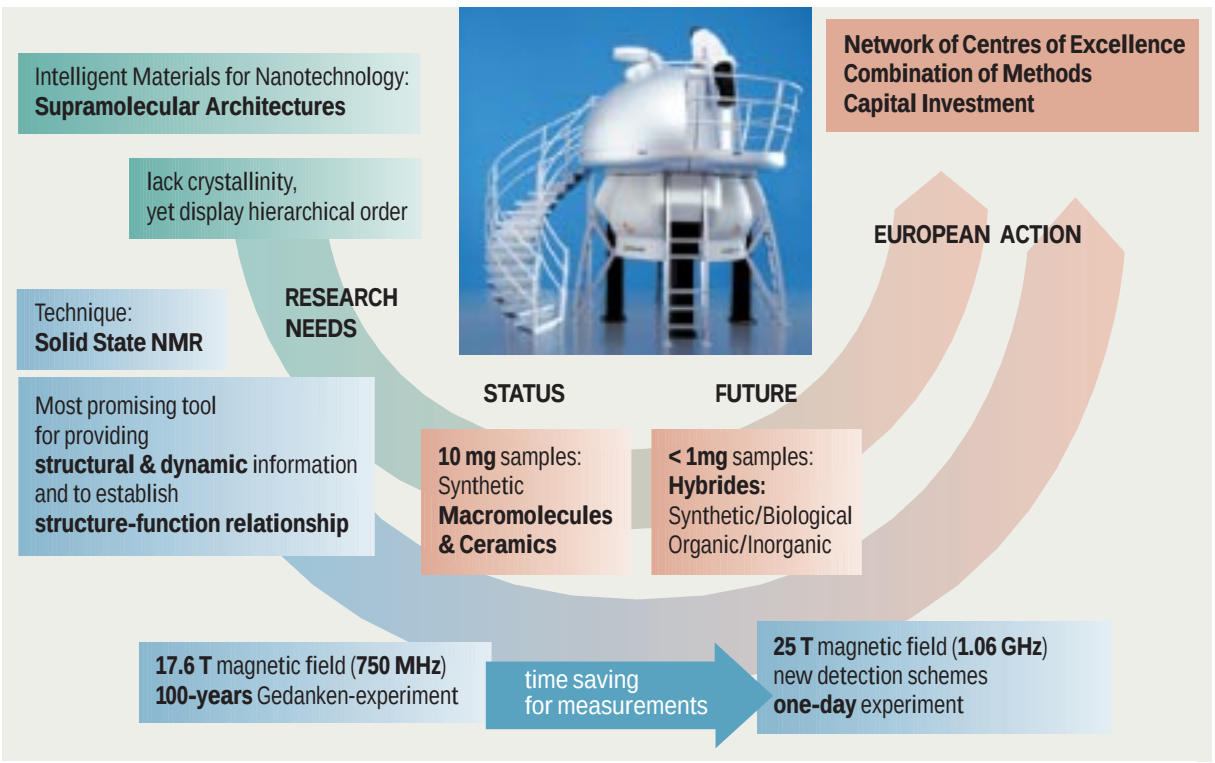

Fig. 7.15. Summarized scheme: How solid state NMR is and will be capable of investigating materials from nanotechnology.

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and high magnetic fields in excess of 16 Tesla (700 MHz or higher) have made it possible to

- locate protons in hydrogen bonds, study their dynamics, and relate these findings, e.g. to thermal rearrangements of smart supramolecular polymers (see Fig. 7.16a) or proton conductivity,
- specify the mutual arrangements of aromatic moieties and relate them to charge carrier mobilities in photonic materials (see Fig. 7.16b), as well as to molecular recognition in guest-host systems,
  elucidate the organization of macromolecules attached to surfaces, identify surface active sites and relate these observations to enzyme encapsulation as well as catalytic activity of zeolites,
- detect unexpected chain order of synthetic macromolecules in amorphous melts & nanostructured materials and relate it to their flow behavior,
- probe the mechanism of generating inorganic / organic hybrid materials, elucidate their structure on various length scales and relate it to their efficient ion conduction.

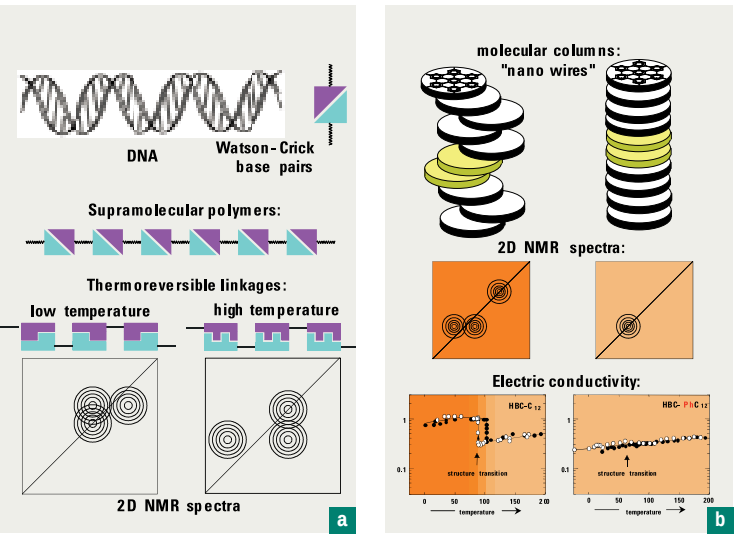

Fig. 7.16 (a) The famous double-helix structure in DNA is based on hydrogen-bonded base pairs. The same principle for structure formation can be used in synthetic polymers, and the linking units can be investigated in detail by NMR, as shown here for the case of a thermoreversible link. **(b)** The electric conductivity in molecular columns, which are candidates for "nano wires", critically depends on the molecular stacking arrangement, which can quickly and in detail be elucidated by NMR spectra.

These techniques require only small amounts of sample, typically 10 – 15 mg, and no special treatment such as single crystals or isotopic labelling. Qualitative results are typically provided overnight, thus the findings of the NMR investigations concerning supramolecular organization can directly be exploited by the synthetic chemist for optimizing structures.

As far as dynamic processes are concerned, multidimensional solid state NMR provides unique information about the geometry, the time scale and memory effects of molecular or ionic motion over an exceptionally wide range of time scales (Table 7.9). Combining solid state NMR techniques with concepts from magnetic resonance imaging, well-established in medical diagnosis, this information can be spatially resolved and related, e.g. to the failure of materials resulting from mechanical overload (shear bands). Solid state NMR is a highly competitive field, with strong activities in the U.S. Most of our colleagues there concentrate, however, on biological systems and almost entirely focus on isotopically labelled samples, an approach not well suited for materials applications. Notably, the group in the U.S., which currently uses the techniques developed in our laboratory most actively, works Europe, but in an industrial laboratory. Solid state NMR in Japan is considerably weaker than in the U.S. and sustained efforts are planned for the coming years.

7.7.3. Expectations and Needs

The development of NMR methods is far from being complete. In fact, in the last decade convergence of the spectroscopic and technical demands on NMR spectrometers is observed. Typical solid concepts as magic angle spinning are now used in high-resolution NMR of liquids. Inverse detection resulting in significant signal enhancements, well-established in liquid state NMR will provide yet another boost to solid state NMR. We recently showed that the sensitivity for such an important element as nitrogen can be increased by a factor of 10 through this approach. Another example is the detection of oxygen, which sofar has largely escaped elucidation by NMR. Even higher magnetic fields will become available, which will provide improved spectral resolution and sensitivity. The next generation of high-field spectrometers in the range of a Gigahertz (23,5 T) will be used with the same magnet for liquids and solids (Fig. 7.15). Major investments, however, are needed to build such a machine.

These developments will enable NMR to handle considerably more complex materials as it is possible today. Such systems will combine different interdependent functionalities which can be triggered externally. Major advances, however, can only be achieved if the development of NMR is intimately intertwined with other techniques of materials characterization, in particular synchrotron radiation and neutron scattering, scanning probe microscopy, UV-spectroscopy and last, but not least computer simulation. This is due to the fact that the structural information

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		Scattering		NMR	
		incoherent	coherent	single quantum	double quantum
Dynamics	Molecular	n-quasielastic		2D-, 3D-, 4D-exchange	sidebands
	Collective		n-spin-echo	2D-exchange	decay of DQC
Structure	Molecular		WAXS, WANS	sidebands	2D signal pattern
	Collective (packing)		pole figures, SAXS, SANS	DECODER chemical shift	2D signal pattern

Table 7.9. Comparison of scattering and NMR techniques as well as the information provided about structure and dynamics of materials.

provided by NMR is not as complete as a full three-dimensional X-ray structure of a crystalline material. For instance, distance constraints provided by NMR will be most useful, if incorporated in the analysis of powder X-ray or neutron scattering data. If a series of compounds is to be optimized, NMR can conveniently check whether related systems exhibit the same or different local arrangements of building blocks. Therefore, in such cases the much larger effort and cost of using large scale facilities such as synchrotrons or neutron sources can then be avoided.

Likewise, computer simulation is indispensable in order to make optimum use of the structural and dynamic information provided by NMR. Both, quantum mechanical calculations of NMR parameters probing the electronic structure beyond a molecule, e.g. the chemical shift of protons in proximity to aromatics or ions and molecular dynamics simulations are required. Major improvements, concerning the size of systems that can be handled are expected during the next 5 -10 years, due to the foreseeable increase in computational power and development of more efficient algorithms. Equally, surface NMR must be closely intertwined with surface specific techniques such as scanning probe and electron microscopy, or synchrotron radiation. NMR, however, is the only technique available which combines clear-cut chemical analytical information with probing the packing of molecules at surfaces

7.7.4. Proposed Actions

• A large scale programme advancing materials science in Europe must include a major commitment to NMR spectroscopy. The emphasis should not be on the development of new NMR techniques as such, but rather to foster interdisciplinary research combining synthesis, characterization, computer simulation and the generation of devices.

• Industry should be included in Co-ordination Groups, assuming rapid transfer of technical advances to industrial laboratories.

Unique expertise in solid state NMR of Materials exists in Europe, e.g. in Switzerland (ETH, Zürich), France (Univ. of Lille), Netherlands (Leiden University), Poland (Poznan University), Germany (Mainz). Moreover, one of the world-leading manufacturers of NMR spectrometers is based in Europe (Germany, Switzerland, France).

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Conclusions

1. Current State

The current state of modern analytical techniques in Materials Science can be considered to be excellent in Europe, pioneering work has been done in the past in the development of X-ray and neutron scattering, in the development of quantitative electron microscopy, NMR and optical spectroscopy. In summary, Europe holds a world-leading position in the advanced analysis of materials.

2. Projects for the Near Future

In the near future novel analytical techniques may emerge with large potential for Basic Materials Science:
(a) New X-ray sources may become available in the near future which are no longer based on Synchrotrons but on Linear Accelerators ("Linac-Based X-ray Sources"). They will provide X-rays with unheard properties, as the so-called X-ray laser (XFEL) which would give, for the first time, the Materials Scientist a fully coherent X-ray pulse at hand allowing time-resolved structural studies in the femtosecond regime.

(b) The proposed European Spallation Source (ESS) with its increased peak intensity will provide novel applications in Basic Materials Science, particularly in the fields of polymer science, magnetic materials and biological systems.

(c) In high-resolution electron microscopy novel aberration correction lenses ("C_S-correction coils") are now possible which give acces to high spatial resolution at significantly lower electron energies. New concepts allow local electron spectroscopy with sub-eV and sub-Ångstrøm resolution.

As a general trend, the classical boarders between diffraction, microscopy and spectroscopy dissappear: With the advent of X-ray micro- and nanobeams local information becomes accessible to X-rays. Already today the strain state of individual grains within a polycrystalline sample can be isolated with the use of X-ray microbeams. TEM can be combined with electron spectroscopy providing element specificity. Shortest and fully coherent X-ray laser pulses would finally permit the materials scientist to obtain holographic images of materials on a femtosecond time scale.

3. Advanced Materials Analysis in Materials Science:

It is somewhat interesting to note that today's standard analytical reservoir of a typical materials scientist encompasses only a rather limited set of analytical techniques, as qualitative electron microscopy, powder diffraction, small angle scattering and EXAFS. NMR, X-ray and electron spectroscopy are also used, essentially as fingerprint techniques. This is contrasted by novel dedicated and highly specific analytical techniques which have been developed in the past years and which could have an enormous potential in basic materials science, but are not exploited today, because they are rather complicated and require an experimental and theoretical training prior to a robust application. Thus, one future challenge in basic materials science is the attraction of materials scientists to Large Scale Facilities which offer sophisticated novel analytical techniques for the investigation of their new materials and material systems. Materials scientists who use these facilities could profit a lot and, as a by-product, can play the role of a catalysor in the (so far rather unsuccesful) attempt of these facilities to attract research laboratories involved in applied materials science and industries to make extensive use of the experimental possibilies offered there.

4. Outlook

Todays materials science and technology is based on our insight into the atomic structure of materials allowing us to compose taylor-made nanosystems with novel properties. In future nanosized materials will continue to play a key role in almost all key technologies. It is somewhat impossible to predict, how materials science and technology will be in 50 years from now, however, as it appears today, it will presumably be based on our understanding and control of the dynamic behaviour of nanomaterials on the femtosecond time scale. This endeavour can only be successful, if new sophisticated techniques will be at hand which allow the analytical access to this new domain of basic materials science.

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5. Necessary Action – Advanced Materials Analysis

It is mandatory that Europe devotes strongest efforts to maintain its leading position in the forefront development and advanced use of new analytical techniques. This know-how is considered to be prerequisite for the understanding of new materials phenomena and for the development of new materials with novel properties. The following European actions are recommended:

(a) European Networks

1. Creation of interdisciplinary networks for the application of Synchrotron Radiation, Neutrons, Electron microsopy, NMR and Laser Spectroscopy in basic materials research.

2. Long-term support of those large scale installations in electron microscopy, NMR and laser spectroscopy which assure access for the European basic materials science community.

3. Creation of Fellowships to foster crossdisciplinary programmes in advanced materials analysis.

4. Creation of long-term "Local contacts for Materials Characterization" at synchrotron and neutron scattering facilities, staffed with experienced personnel (scientists, engineers) as the primary contacts for materials researchers from the different institutions and different research fields in Europe.

(b) European Centres of Excellence

should be created in:

1. Synchrotron radiation for basic research in materials science
2. Neutrons for basic research in materials science
3. TEM Analysis
4. NMR Analysis
5. Laser Spectroscopy (in particular ultrafast spectroscopy)
6. Advanced analysis of surfaces, interfaces and nanomaterials
7. Structure analysis of biomaterials

(c) Resources

The development and construction of new dedicated instrumentations for advanced materials analysis which require larger investments (> 1 Mio Ecu) has to be supported on a European level. Particular focus should in the development of innovative analytical techniques which carry the potential to unravel new time and length scales and which are of interdisciplinary use. The Centres of Excellence listed in **(b)** should coordinate such enterprises and the later use of such new experimental stations by the European materials science community.

(d) Training

1. Creation of fellowships for doctoral students, postdoctoral students at large scale facilities.

2. Creation of mobility programmes for young scientists and for achieved experts to support flexible stays at large scale facilities.

3. Support of European Workshops and Conferences in "Advanced Techniques in Materials Characterization"

(e) European Advisory Boards

A European advisory board is strongly recommended which coordinates the Synchrotron Radiation and Neutron Activities in Europe.

(f) European Large Scale Facilities

European support is recommended for the new initiatives to build the new-generation facilities, in particular the European Spallation Source (ESS) and the 1 Ångstrøm-X-ray-Laser (XFEL), which carry the potential for future breakthroughs in materials science.

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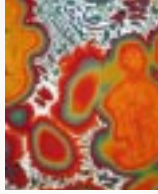

8. Materials Science in Europe

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8.1. The Importance of Materials

All modern societies are experiencing a profound change in their social and economic structures. As technology marches forward, many traditional occupations are disappearing, while the number of people working in high-tech occupations is increasing. There is no doubt among politicians and their advisors that the economically strong societies of tomorrow will be based on knowledge and technological skills, particularly in regard to

- energy and environment,
- medicine and health care,
- mobility and transportation,
- information and communication.

These have been recognized as the key technologies that will determine the future welfare of society. It has also been realized that any progress in these technologies critically depends on the development of new and tailor-made materials with improved or novel properties, e.g., new biocompatible materials for medical applications, and opto-electronic materials for computers and communication devices. Pressure to improve and protect the environment means that recycling issues will affect almost all fields in which new materials are produced.

Modern high-tech materials are prerequisites for all major research and development areas, from space programmes, astronomy, and particle physics, to modern surgery, computing, and fuel cell research. While all these technologies rely on the precise and dependable performance of specialized materials, the role of materials science is often not appreciated by the public because its activities generally take place in the background. For science to continue to develop materials for new technologies in the future, however, a greater appreciation of its importance to economic growth and social prosperity is needed. New materials and materials systems with improved performance and previously unimagined properties are essential if European industry is to remain competitive and a high standard of living is to be guaranteed for more people well into the 21st century.

From high school science we have learnt to associate a given material with certain characteristic properties, such as electrical conductivity, specific heat or melting temperature. As our ability to control the structure of materials has now been extended to the nano-scale (around 10^{-9} m), however, we have come to realize that the behaviour of a material can be significantly different when confined to extremely small sizes. These “nano-properties” are mostly due to the high surface-to-volume ratio of the particles, but they can also result from the limited extension of the system, as many “bulk” properties are collective phenomena averaged over relatively large length scales (typically µm or greater). Consequently, novel effects not seen in nature can be created by designing materials at the nano-level. Nanostructures also test our theoretical understanding of what happens when systems become very small, lying – as they do – at the border between classical and quantum physics. Common examples of nano-

◀ Optical micrograph of a colour etched CuSn10 cast (G.Kiessler, MPI für Metallforschung Stuttgart).

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designed systems are thin semiconductor and metal films, which exhibit unusual electrical and magnetic behaviour, and colloidal systems that are already in use today, e.g., titanium dioxide (TiO_2) nano-particles in sunblock creams. More exotic structures and phenomena are now becoming the focus of scientific interest, e.g., confinement of liquids within nano-sized slits to understand how friction and lubrication behave in the nanoworld.

New theoretical concepts are needed to model these structures, and new analytical tools are required to observe *in situ* the behaviour of atoms and molecules in confined space. This is a very active research area for materials scientists, and we can confidently predict that some of these phenomena will become the new technologies of tomorrow. Richard Feynman's inspiring statement more than four decades ago that "there is plenty of room at the bottom" is now being proved true. This new world of nanomaterials is being made possible by continuous advances in instrumentation and analysis, which allow us to build materials atom by atom and will in future enable us to observe molecular motion on femtosecond (10^{-15} s) time scales.

In the next decade the development of materials and discovery of new phenomena will be strongly influenced by interdisciplinary approaches involving numerous scientific and engineering fields, including condensed matter physics, chemistry, biology, computer science, and materials, chemical and mechanical engineering. Successful collaborations between materials scientists and medical scientists to create biomaterials, and between condensed matter physicists and biologists to create soft condensed matter (materials that are easily deformed by external stresses, electromagnetic fields or heat), indicate that such multidisciplinary research projects have a bright future.

Another consequence of interdisciplinary research projects is that future materials will become progressively "smarter"; in other words, the materials of tomorrow will actively communicate and respond with their environment. Packing materials will be able to sense the state of the contents, the superstructures of aeroplanes, trains, ships and cars will be able to detect microcracks and provide early warning of any problems. "Smart coatings" will be able to repair themselves if damaged or attacked by corrosion. Computer chips will become as small as grains of dust ("smart dust"). It is also envisaged that materials will be created which self-organise to form large complex units with controllable properties. Organic memory for the computers of tomorrow may be built using special-purpose bacteria as "microbe-factories". The possibilities are seemingly endless.

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8.2. The Role of Basic Materials Science

Our skills in materials technology today are such that we can control the properties of condensed matter at the atomic level. Today's insights into the atomic structure of materials and our understanding of the rules that control materials behaviour date back to the beginning of last century, when the laws of quantum mechanics were expounded and when X-ray diffraction opened up to us the internal structure of matter. The main motivation for these scientific achievements was scientific curiosity, and the human instinct to seek to understand the world around us.

As a result of these fundamental discoveries in basic science, new technologies were born, and a new type of research emerged, applied research. Applied science, together with engineering, has been very successful in improving and tailoring materials and phenomena for use

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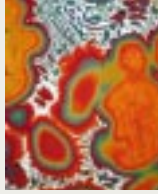

in real world applications. This **evolutionary** approach employed by much of applied science leads to improved performance of materials and devices in a more-or-less predictable fashion. A textbook example is the continuous miniaturisation of integrated circuits (ICs) in accordance with Moore's Law, which states that the number of transistors on an IC will double approximately every 18 months.

Applied (i.e., evolutionary) materials science extends scientific understanding through incremental and predictable developments. Such applied technology is often the province of industrial research, which seeks to extend the commercial capabilities of existing materials through lower cost, longer life, and more consistent and reliable products. On the other hand, it is also known that this evolutionary approach is fundamentally limited and cannot solve the challenges in materials science that will confront us the day after tomorrow. In order to tackle these problems, new, **revolutionary** approaches in basic science are needed. In this case, we should not aim for incremental improvements in known materials and phenomena so much as embark on a search for new materials and phenomena. Such research projects should in future be based at universities and materials science research institutes throughout Europe, and initiate most of the curiosity-driven, pre-commercial materials research.

Unfortunately, a feature of basic scientific research is that its results are unpredictable, i.e., neither the success of a project, nor the time required before positive results will be forthcoming, can be forecast in a reliable way. In addition, it happens only rarely that a fundamental discovery leads immediately to a new product. Rather it may take many decades to produce “spin-offs” in the form of novel applications and innovations. This fact lies behind why basic science is often criticised or neglected; namely, that most of the announced “scientific breakthroughs” never seem to become new, useful technology. This “conflict” between curiosity-driven science and the current needs of society is as old as science itself. One need only recall the famous encounter between Faraday and King William IV, who once asked the celebrated scientist what “his electricity” was actually good for. Faraday answered, “One day you will tax it”.

Curiosity-driven basic science has revolutionised many old technologies and even sparked new ones in the past, e.g., the accidental discoveries of glass-ceramics with zero thermal expansion at Corning Labs, U.S., in 1952, and electrically conducting polymers in the 1970s at the University of Tsukuba, Japan. In some cases, materials breakthroughs have a direct impact on current technologies, e.g., the discovery of the giant magnetoresistance (GMR) effect in 1986 by Grünberg at the Jülich Research Centre now used in modern read head technology. In other cases, such as high temperature superconductivity (discovered by Bednorz and Müller, also in 1986), unforeseen technical difficulties mean that more time is needed to turn the enormous potential of superconducting ceramics into affordable, reliable products. In the fifteen years that have elapsed since the initial breakthrough, however, substantial progress has been made, and we can expect to see the first useful applications of these amazing materials within the next few years.

By its nature, basic research is best carried out at universities and national research laboratories, where commercial interests can be set aside. Having said this, close contact with industries that have an interest in the research, or are seeking solutions to materials problems, can benefit both sides through the exchange of ideas and inspiration to innovate. Basic research at universities therefore has the dual role of increasing knowledge for the benefit of individuals and society, as well as helping solve problems of industrial relevance and sowing the seeds for new technologies.

The synergy between university-based and industry-based research teams has been an important factor in the success of U.S. materials research, exemplified by the excellent laboratories established by DuPont, IBM, AT&T, Corning and Exxon. These laboratories have produced several Nobel Prize winners, not least of all Bardeen, Shockley and Brattain in 1956 for the discovery of the transistor effect. This successful tradition has, unfortunately, never been developed in Europe and has also now essentially been abandoned in the U.S. Many European companies have eliminated corporate or central research laboratories to more closely align research and development with immediate business opportunities. Furthermore, there are strong economic incentives to turn exploratory research directly into new products. This commercialisation may require researchers in industry to focus their efforts on resolving market-related aspects of product/process development at the expense of fundamental materials understanding. The pitfalls and hazards of this rather non-sustainable approach are manifold (e.g. in the form of materials failure or undetected hazardous side-effects).

Future breakthroughs in materials-based technologies can only be achieved in Europe when the central role of basic science in the search for revolutionary new materials and phenomena is recognised by the European Community. It is critical that new and sustainable programmes in basic materials science research are launched to form a reliable

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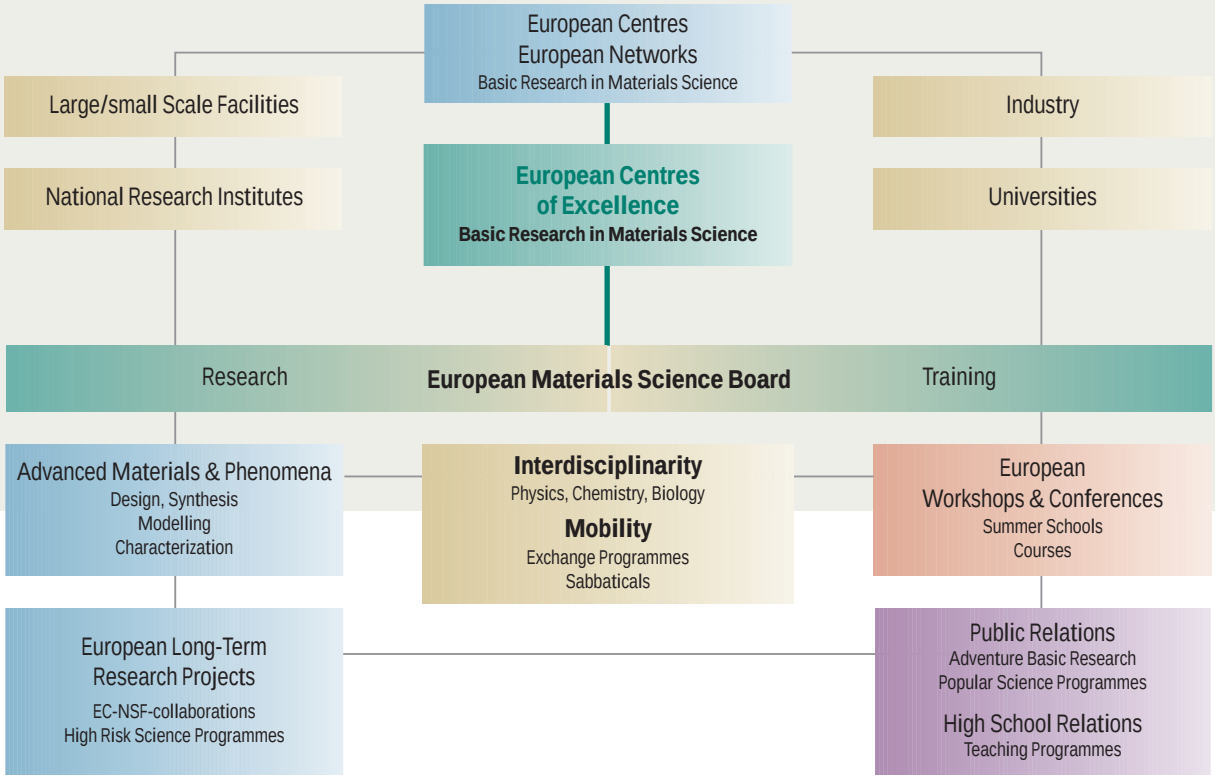


Fig. 8.1. European scheme of basic research in materials science.

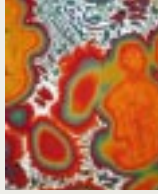
backbone for European materials science networks and materials science centres. The schema proposed in Figure 8.1 highlights the role of basic research in materials science and development in Europe (see also Sect. 8.6).

The unquestionable triumph of materials science during the past century, which improved our lives immeasurably, may be ascribed to the successful search for elegant solutions to complicated problems. This strategy must be continued in the future and include new elements such as rapid information exchange and interdisciplinarity. The new millennium will see us enter an era of novel materials complexity. With new tools, new insights and understanding, and a developing convergence of the disciplines of physics, chemistry, materials science, biology and computing, we may dare to dream of novel and superior materials properties that were, until the 21st Century, the stuff of science fiction.

8.3. Social Acceptance of Basic Science

Today we take for granted the fact that new high-tech products appear on the market almost continuously. This has led to the rather deceptive attitude that no effort need be put into research for the next generation of technologies, as they will appear from somewhere else in any case. For young people it is even fashionable to be firmly against modern technology and new technological developments, while simultaneously relying on advanced telecommunications, transport and medicine for their daily lives. The natural sciences have steadily decreased in popularity all across Europe, particularly among young people, who typically associate physics with Chernobyl, radioactive waste and nuclear weapons, chemistry with oil spills, polluted air and poisoned rivers, and biology with mad-cow disease, gene-manipulated organisms and cloning.

It is difficult to deny that basic science has lost much of its prestige and trustworthiness in the public eye. This is due



in large part to the erosion of the traditional framework of disinterested, independent research at universities, and its replacement by a complex association of public, private and industrial laboratories, often with commercial goals. Ordinary citizens are more likely to question the validity or usefulness of an innovation when vested interests are at stake, so that people are much more cynical about the role of science as the final arbiter of truth than they were thirty or forty years ago. At the same time, scientific breakthroughs are having a larger, more rapid and more profound impact on society than at any other time in history. Without scientific progress, Europe will be unable to compete economically or culturally with the rest of the world, and many of the problems that we now face will grow in magnitude until it is too late to fix them.

One of the unfortunate consequences of these trends is that many talented young students choose to study law, business or accounting rather than science. This dangerous "internal brain drain" has developed because scientists have failed to communicate the relevance and risks of their research to the wider public in a convincing manner. It is also true that the priorities of science and the rest of society have diverged over the last two decades. A profound change in society's perception of basic science and its importance for Europe's future welfare is therefore required if opposition to scientific progress is to be reversed. It is imperative that materials scientists make every effort to convince politicians and the younger generation that

- the current prosperity results from scientific knowledge obtained through intensive research over the last century,
- tomorrow's technology cannot be created by simply extrapolating the current knowledge.
- only through the application of science and rational-thinking it is hoped to solve today's problems in a satisfactory way.

It is the responsibility, and indeed duty, not only of materials scientists, but also of all scientists, to restore the confidence of the general public in our ability to create a better future. Public understanding of science is important not only so that scientists can discuss their research with lay people (thereby, hopefully, receiving their support), but because without a better understanding and appreciation of science it will be impossible to maintain the culture of inquiry and open-mindedness necessary for a knowledge-based society. There is an urgent need for open dialogue between scientists and other groups in society, including representatives from national and European parliaments. Materials scientists must be more willing than has been usual in the past to educate the public about the fascinating adventure that they are involved in, and the manifold benefits that materials science brings to society. Science must become embedded in a long-term political framework that provides a sense of security and a positive vision for the future.

The first step in effecting a "sea-change" in science-society relations is through better education. This will require better training of teachers in science for high schools, and include a larger science component in the training of elementary school teachers. It is also important to provide better access to science education for mature students, perhaps through the Internet, or other "virtual" university schemes; the Open University in the UK is one such example. University science courses should also include humanities components such as ethics, philosophy and history. This would help produce well-rounded science graduates with improved communication skills and an appreciation of the concerns and ways of thinking of other members of society.

Some other practical suggestions for improving the public understanding of science include (see also Sect. 8.5 and 8.6):

- European Science Summer Events organised by European Centres for Materials Science in collaboration with high schools (see also Sect. 8.6). These could be along the same lines as the National Science Week activities sponsored by the British Association in the UK,
- high school curricula should be updated and modernised to include the latest discoveries in science and technology. It is essential that the excitement and wonder of science be conveyed at an early an age as possible,
- talented high school students could be offered internships in research laboratories during summer or winter vacations as part of their studies,
- the training of science teachers should be updated to include the latest knowledge, and bridging and refresher courses offered to high school teachers,
- closer ties between universities and high schools should be established, perhaps by offering fellowships to talented and motivated science teachers,
- writing of popular books on materials science and its fundamental importance to many technologies should be sponsored, so as to give materials science a higher public profile.

Possible initiatives to be taken and/or supported by the European Commission include

- popular science programmes on TV that focus on the latest developments in solid state physics, chemistry and materials science

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- open days at research institutes with stimulating presentations of current research and
- popular science articles that focus on current challenges and achievements in basic research in materials science.

Science and its application have numerous social, cultural, moral and philosophical dimensions that we need to take into account, whether as guides to our own actions or to better understand the actions of others. The public's trust in science cannot be re-established until scientists learn to take into account value-laden world views (both their own and those of others) when discussing scientific issues. It is important that materials scientists be more willing to engage the public in discussions and debate, not only as "experts" with facts to convey, but also as individuals with opinions and concerns of their own who can work with others to solve problems. More inclusive, less adversarial means of communicating with non-specialists need to be set in place to cope with the far greater diversity and pluralism of today's postmodern society. Only by giving the public a say in which directions research heads, and the uses to which it is put, will science regain the confidence of the broader public.

Although materials science does not experience the same degree of opposition as, for example, some of the biological sciences, there are still several issues of public concern that materials scientists need to keep in mind, as recycling issues or concerns regarding military use or misuse of materials (e.g. data protection) .

Many of these issues also touch upon areas in the mining, minerals, construction, and manufacturing industries, which have close ties to materials science. In this era of mounting environmental concern, it is therefore incumbent upon materials scientists to promote the use of environmentally benign technology, e.g., non-polluting energy sources, "cleaner" materials processing, and composites made from natural fibres. This is one area in which collaboration between scientists doing basic research and industries seeking "greener" methods can reap huge rewards.

Science has been well embedded in our culture and way of life, but to ensure that this remains so, scientists must learn to listen more attentively and talk more transparently to the public. In this age of increasing globalisation, science must be seen to be of benefit to the underprivileged and not just a means of profit for the privileged. This is especially true if it is to regain acceptance as a force for good in the eyes of a large fraction of today's society.

8.4. The Interdisciplinarity Challenge

Materials science has been very successful in the past, providing us with a variety of high-performance materials that have laid the foundations for modern technology. Most of this progress has been accomplished by staying within well-established, somewhat isolated fields, such as semiconductor technology, metallurgy or advanced ceramics. These days, materials science is more and more about developing a multidisciplinary approach to research in which physicists, chemists, biologists and engineers all contribute. Typical examples are surface science projects and nanotechnology, neither of which would be possible without collaborative links between disciplines. We will increasingly find in the future biological molecules being incorporated into inorganic materials with tailored functions (for example, in sensor technology and in nano-motion research), and theoretical and analytical concepts from materials science being used in biology. While difficulties can arise when scientists from different backgrounds try to communicate (because of different terminology, concepts, aims, etc), the potential synergies of such interactions have only partly been explored and their importance cannot be overestimated.

Very often new and fruitful ideas come from young minds not yet set in the established, discipline-oriented way of thinking, or when experienced scientists change from one field to another. It is therefore important to encourage greater exchange of students and scientists between disciplines. One way of achieving this is by ensuring that economic and administrative barriers do not prevent movement of scientists from one discipline or country to another. In Europe, this would be aided by standardised qualification recognition procedures, European-wide training courses, and official exchange programmes (see Sect. 8.5). An interdisciplinary culture must also be implanted through educational (universities, research institutes) and

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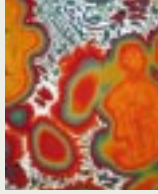

budgetary (funding agencies, national governments, European Commission) initiatives. It must also be realised that the heterogeneity of European culture is an asset with the potential to provide imaginative ideas and diverse skills that must be more efficiently utilised in the future.

High schools and universities tend to be rigidly structured around scientific disciplines, thereby rendering transfer between disciplines difficult. This problem was realised some years ago by German physics departments, which now offer optional one-term courses in business and even in art (so-called "soft skills"). This, however, does not deal with the materials science issue addressed here. In order to provide a more interdisciplinary education in the natural sciences, it is tempting to replace physics, chemistry and biology courses at schools and universities with courses on "natural science" so as to convey a more unified, less fragmentary, view of science. The danger is, of course, that this could easily result in graduates who understand a little bit from everything but nothing in depth. Care must therefore be taken to ensure that students are given the opportunity to specialise just at the right age or educational level where they have sufficient background knowledge of all the sciences.

One way of promoting a multidisciplinary approach to materials science is to offer students in different disciplines (physics, chemistry, biology, engineering) from all over Europe the chance to attend an intensive four-week training course in a field of advanced materials science (during their summer vacation, for example). These summer training courses should end with an assessably written or oral exam. Students who successfully complete the course could be given a suitably named "diploma", which would then become a prestigious qualification that raises the employability of students in the eyes of industry. In order to ensure the success of this scheme, we recommend the following measures to be taken by the European Commission:

- use a rigorous procedure for selecting students,
- solicit the best researchers in the field to run the courses,
- hold courses at attractive locations that provide an invigorating environment for study and
- include plenty of free time for discussion and other activities, in a manner similar to the successful Gordon Research Conferences.

Further strategies for fostering interdisciplinary scientific communication at all educational levels, from high school to university to postdoctoral training at research institutes, include:

- establishment of university courses in interdisciplinary areas, e.g., biomaterials courses offered by materials science departments in conjunction with biology departments,
- modern student textbooks on aspects of interdisciplinary research that should be written by acknowledged experts in materials science,
- summer Schools for Interdisciplinary Science, which should be organised by European Centres of Excellence (see Section 8.6) for graduate and postgraduate students as well as selected high school students (based on academic excellence or scientific aptitude),
- European workshops and conference series focussing on the multidisciplinary aspects of materials science; these should be organised jointly by universities and European Centres for Materials Science and Technology (see Sect. 8.6) and be particularly open to students and scientists at the beginning of their careers.

European funding agencies, national governments and the European Commission should foster multidisciplinary studies by

- providing financial support for the European workshops, conferences and summer schools mentioned above,
- supporting multidisciplinary materials science research programmes,
- supporting the establishment of interdisciplinary research centres (IRCs) and facilities (see Sect. 8.6),
- encouraging agreements between agencies that fund research in different disciplines to better coordinate multidisciplinary research efforts,
- granting fellowships and startup money to scientists taking their expertise from one field to another and
- encouraging researchers in Europe to spend time in other countries and laboratories, i.e., improve researcher mobility (see Sect. 8.5.3).

European centres for materials science and technology (see Sect. 8.6) should take a leading role in promoting interdisciplinarity by assembling diverse teams of researchers from materials science, physics, chemistry, biology, computer science and engineering in order to tackle high profile and relevant scientific problems. This is the philosophy behind the IRCs established in the UK recently, such

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as the IRC in Polymer Science and Technology at the University of Liverpool, and the IRC in Superconductivity at the University of Cambridge.

The enormous potential of the Internet (and its descendant, the Grid) for facilitating cooperation and communication over large distances should also be exploited. A register of scientists and engineers working on materials-related research could be established to provide easy, European-wide contact with experts in any given area of materials science. e-Networks such as the MatNet project being developed by the Federation of European Materials Societies (FEMS) should be supported, expanded and emulated.

8.5. New Schemes for Education, Research Careers and Researcher Mobility

Up until less than thirty years ago, scientists working in the fields of physics, chemistry and biology were highly regarded, and even esteemed, by the public at large. Only twenty years ago one of the chief career goals of high school students was to become a university professor in physics, mathematics or chemistry. This picture has changed dramatically over the last two decades as public funding for science has decreased and the implied "social contract" between scientists and the public has been questioned in the postmodern age (see Sect. 8.3). Today, the exact sciences have lost their lustre as the intellectual and innovative determiners of the future, many graduates turning instead to "dotcom" companies and investment banking because of the much more attractive salaries they offer. In order to reverse this dangerous trend, we need new schemes in education, a mechanism for promoting and upholding high ethical standards for scientists, attractive career opportunities for researchers and lowered barriers to researcher mobility within Europe.

8.5.1. Science and Education

The attractiveness of the pure sciences to the younger members of society, such as elementary school children and high school students, needs to be restored, since they will be the future thinkers and opinion makers. We must make every effort to ensure that once again the best of them choose careers in physics, mathematics, chemistry and engineering, rather than business and stock trading. This is a rather difficult task and requires action on many levels, by national governments, professional societies, institutes and individual scientists.

It is also important to consider the curricula of elementary and high schools, which tend to concentrate increasingly on the liberal arts at the expense of the hard sciences. While the importance of the humanities and social sciences is undeniable, we need to devote an equal amount of time to physics, chemistry and biology, as well as engineering and computing, without extending the education period further. In fact it has been suggested that, by optimising class content for both liberal arts and the natural sciences, the amount of time spent in school could actually be shortened.

It is clear that teachers in primary and secondary schools cannot tackle this task alone, but need assistance from universities, research institutes and industry. Many scenarios are possible, limited only by the imagination of the organisers. They range from

- public evening lectures,
- open days at research labs,
- visits by young and motivated researchers to schools to convey the excitement of science and a scientific career,
- training seminars for teachers.

At a European level such efforts can be complemented by various European science events, which should be open to all. Among the possible events that could be organised by the European Materials Science Centres are

- visits to large-scale research facilities,
- summer schools on selected topics in materials science,
- practical courses during the holiday periods at foreign research labs.

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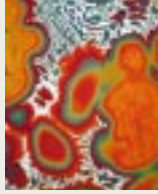

All these events should have a strong international dimension, i.e., many young people from different countries should be encouraged to participate and share their thoughts and experiences. These European-wide excursions should be available first of all to those primary and secondary schools within Europe that have already taken part in some of the local science activities listed above.

8.5.2. Careers in Materials Science and Basic Research

Public esteem for science and the attractiveness of a scientific career must be re-established. This will require effort from all sides, political, academic and industrial. It is regrettable that many excellent materials scientists choose to take jobs with lower qualification requirements in order to secure a decent salary. If this continues, Europe will be forced to rely on scientists from outside the region for its future welfare.

In order to attract talented young people back to basic science and research, fundamental changes in research administration and academic career structures are needed. Most jobs in academia can no longer compete with the career opportunities currently offered by the private sector and this situation will become even worse in the future if no action is taken. It is evident that European universities and research laboratories need:

- more flexibility in hiring people;
- more competitive salaries;
- more attractive career options for young people;
- more women students and lecturers/professors.

The establishment of new, prestigious awards at various levels (graduate, postgraduate and senior researcher) for outstanding achievements in basic and applied research, sponsored by the EC, would also serve as an incentive for more people to take up careers in materials science. These could be named after famous European scientists who laid the foundations for modern materials science.

The difficulty of obtaining university tenure and the long years of waiting in low-paying, non-secure postdoctoral positions beforehand often discourage students from choosing careers in academic science. Measures should therefore be set in place that encourage universities to recruit more people to permanent positions, rather than increasing the number of postdocs. Part of this problem could be relieved by an active campaign to attract more students (particularly female students) to materials science, thereby creating a need for more teachers.

In addition, the versatility and intellectual preparedness of students must be increased without increasing the MSc or PhD study time. Materials science graduates must continue to receive a comprehensive grounding in their field along with quality research experience, but at the same time career guidance should be provided to expose them to other fields of endeavour. To improve the employability of materials science graduates and postgraduates, increased emphasis should be placed on developing those qualities which industry is looking for in new recruits, namely problem-solving and communication skills, leadership potential, and the ability to work in multidisciplinary teams. Students should also be imbued with a more entrepeneurial spirit for commercialising and selling their innovations. These skills are useful not only for a career in industry, but also for boosting the confidence of students in their ability to communicate with specialists and non-specialists alike. It is also important that students be encouraged to continually update and extend their skills once in the workforce through professional development programmes and personal study and/or training.

8.5.3. Researcher Mobility

Science cannot exist without the constant and direct exchange of knowledge and ideas within the scientific community. The publication of scientific results and the organising of conferences and workshops are, thus, indispensable ingredients for scientific productivity. Science has become so complex that progress also requires scientific exchange on a broader level.

A barrier to the efficient use of European scientific talent is the lack of mobility of scientists at all levels (from undergraduates to university professors). Movement of undergraduates and graduates within the EC is severely hindered by the different education systems in each country. Language problems and cultural differences can also add to these difficulties.

Increased mobility of junior and senior European researchers should be seen as a priority for the EC to broaden scientists' experiences, foster greater cross-fertilization of ideas and disseminate new findings and methods as rapidly as possible. One way of promoting greater mobility within Europe would be to establish a standard qualification for European Materials Scientists (EurMat) similar to the European Physicist (EurPhys) qualification granted by the European Physical Society. The EurMat qualification could be awarded by the Federation of European Materials Societies (FEMS) on behalf of the EC and would be

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recognized throughout Europe as indicating a certain level of academic attainment and professional experience had been achieved by the bearer.

Another way of improving researcher mobility would be by awarding European Studentships and Fellowships in Materials Science to people at all levels of education and experience (i.e., undergraduates, postgraduates, young and senior researchers, research directors and university professors). It is important that the Studentships/Fellowships be administered by only a few leading materials research authorities via a flexible, efficient and non-bureaucratic selection process based on ability and aptitude. European research institutes should be encouraged to apply for European Host Fellowships that allow them to select talented students and researchers for higher-level training and sabbatical stays. The amount of the awards should be suitably high in order to make them as prestigious and competitive as possible. Means of encouraging greater researcher mobility are discussed in more detail in the proceedings of the "Investing in Europe's Human Research Potential" conference held on Crete, Greece in October, 2000.

8.6. European Centres and Facilities for Materials Science

8.6.1. European Facilities for Materials Science

In order to build up a modern European research infrastructure for Basic Research in Materials Science, the existing European research facilities have to become involved and, if necessary, new facilities or research networks have to be created. Fig.8.2. gives a more detailed presentation of a possible European infrastructure.

(a) Large-scale facilities

Modern materials research requires access to radiation sources for probing atomic and electronic structures, which can only be generated by large, expensive equipment located at central facilities. Several such facilities are currently in operation in Europe; e.g., X-ray and neutron facilities are provided by the European Synchrotron Radiation Facility (ESRF) and Institut Laue-Langevin (ILL) in Grenoble, France, and ISIS at the Rutherford-Appleton Laboratory in Didcot, UK. To guarantee Europe's leadership in materials science, several actions are necessary, including:

- increased access to these facilities for materials scientists from all over Europe;
- establishment of new large-scale facilities.

Large-scale research facilities can also serve as a focus for the European materials science community, so that a "critical mass" of researchers can be gathered for making breakthroughs in new and challenging fields. Establishment of large-scale facilities will also help make European materials research more efficient by allowing researchers from different countries to work together, thereby reducing unnecessary duplication of research and exploiting the potential synergy that comes about when researchers from different cultures and backgrounds interact. These facilities will also give researchers from smaller Member States the chance to use large-scale equipment that they would not otherwise have access to.

These facilities should provide scientific services to universities, research institutes and industry throughout Europe, and have sufficient numbers of engineers and technicians to operate and develop them to their greatest potential. In addition, access to these large-scale facilities should be based on a flexible research proposal system. Competitive salaries and working conditions should be offered to attract the world's best scientists, and sufficient funding (through government support or providing chargeable services to industry) provided to ensure that the equipment remains state-of-the-art. A European Materials Science Board (see Fig. 8.1. and Fig. 8.5.) should be created to organize and oversee large-scale experiments, select the most promising and imaginative research proposals, and guide long-term planning/strategies in materials research.

(b) Small- and medium-scale facilities

Small- and medium-scale facilities are also necessary for a vibrant research environment. These should be distributed throughout Europe, including places geographically isolated from larger facilities, in order to maintain diversity and lessen the "brain drain" from the smaller European countries to more favoured regions. They should also be located or under the supervision of experienced research managers who are acknowledged authorities in their field.

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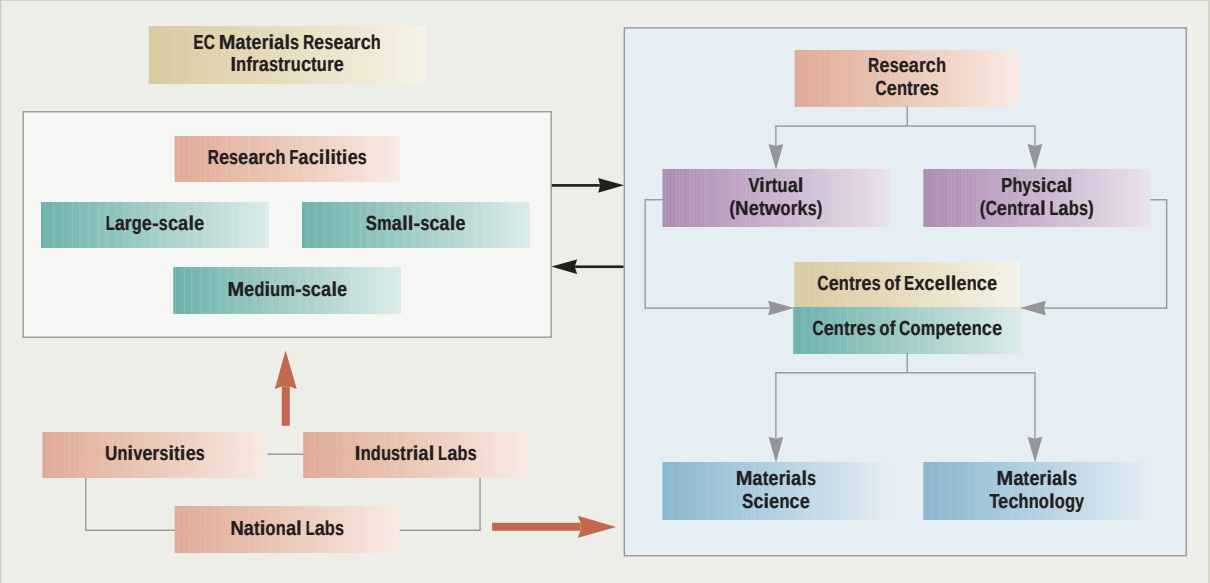

Fig. 8.2. Schematic representation of the infrastructure necessary for advanced materials research in Europe.

Small-scale facilities should be devoted to a single area of materials research, such as electron microscopy, surface analysis (ESCA, Auger), scanning probe microscopy (STM, AFM, STS), crystal growth, optical characterization or advanced materials synthesis and processing. These facilities could be established from funds available from the EC, where the benefits of such facilities to EC projects or networks can be demonstrated. Private industry should also be encouraged to give grants or equipment for the establishment of such facilities in order to promote fundamental research in the areas in which they are interested, and draw from the wider pool of expertise in academia. Such facilities can already be found in many universities throughout Europe, but in some cases there is an urgent need to replace or upgrade old and outdated equipment.

Medium-sized facilities established in conjunction with universities or at research institutes are ideally suited for interdisciplinary research, for example, nanomaterials, biomaterials, advanced composites, and computer modelling. These facilities, and the centres that house them, should have a wider variety of equipment and techniques available than the small-scale facilities. They should be funded both by private companies and government agencies, and should be available to all participating departments in the home university or institute, as well as sponsoring companies and researchers from other public research centres, preferably as part of a wider researcher network.

8.6.2. European Centres of Competence in Materials Science

To focus efforts on materials science in Europe and to gather a critical mass of researchers for making major breakthroughs, Materials Centres of Competence should be established in Europe. These should be Europe-wide and interdisciplinary, and conduct cutting-edge research at undergraduate, doctoral and postdoctoral levels. They should preferably be located near or at large- and medium-scale research facilities or national institutes, or alternatively, exist as "virtual" centres formed from networks of materials science laboratories around Europe (see Sect. 8.6.4). Their mission should be to pursue world-class research into materials synthesis, characterisation, and processing in areas with great potential, including new applications and technologies, and to coordinate research in the public and private sectors.

These EC-funded research centres, also referred to as Centres of Competence in Materials, should have a European-wide mandate with the necessary status and support to effect real change in the way materials research is conducted in Europe.

Both regular "brick-and-mortar" centres and "virtual" centres should be created to satisfy the diverse needs of the materials science research community and provide optimum benefits for Europe. These two types of organizational strategy can be summarised as:

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1. European research centres providing a geographical focal point for investment in infrastructure (large- and medium-scale facilities) and for achieving a "critical mass" of experts in the field of materials.

2. Virtual research centres formed from a network of highly specialised research institutes and laboratories formed by connecting several catalysis groups from around the EC via a broadband communications network.

The centres should be linked by the latest high-speed communications technology, including data transmission and video conferencing, as part of an overall European-wide communications network.

Centres of competence should also be distinguished according to whether the main emphasis is on fundamental or applied research:

(a) European Centres for Materials Science

These centres should seek to perform fundamental research into materials and provide a stimulating environment for physicists, chemists, biochemists and materials scientists to work together. These centres should specialise in one or more of the research fields listed in Fig. 8.3, (i.e., newly established, interdisciplinary and innovative research areas).

These centres should collaborate closely with universities:

- to establish high-quality research and training programmes,
- to organise European workshops and conferences,
- to investigate the potential of new materials and processes for practical applications.

(b) European Centres for Materials Technology

These centres should conduct interdisciplinary materials research with emphasis on materials applications and support scientific exchange and secondments with industry. The main research areas they should cover are listed in Fig. 8.4. These centres could also serve as "incubators" for venture companies exploiting advances in materials technology. Another important task would be to provide training in entrepreneurial and management skills for scientists in conjunction with universities and businesses, including how to apply for patents and license technology to other firms.

The key to the success of the Centres of Competence in Materials Technology will be close collaboration with industrial partners:

- to test and develop new materials applications,
- to mediate the exchange of materials technology between universities and industry,
- to nurture new businesses and spin-off companies based on materials breakthroughs,
- to organise workshops and technology fairs promoting new materials technology.

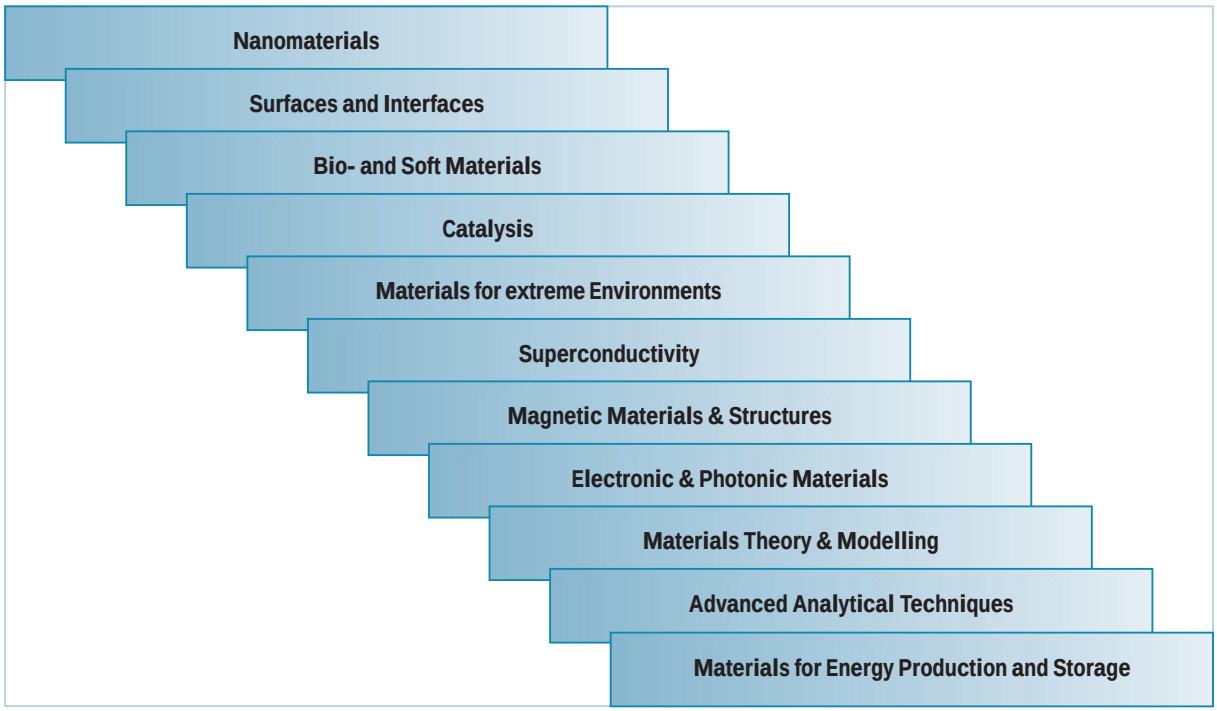

Fig. 8.3. Suggested subjects to be covered by different European Centres or Materials Science.

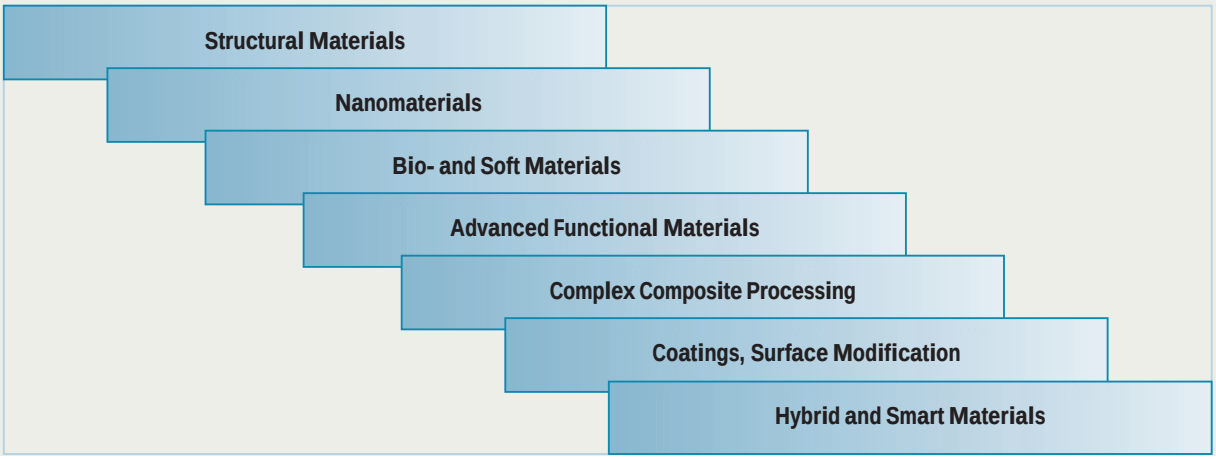

Fig. 8.4. Suggested subjects to be covered by European Centres for Materials Technology.

Centres of Competence should offer fellowships to top-class applicants from each sector (industry, academia and government labs) to work on European materials projects. Permanent research staff drawn from all three sectors should also participate in these projects, as well as support the wider range of tasks listed above. Materials Science and Materials Technology centres should also maintain close links with each other so that the entire gambit of materials research, from fundamental studies to industrial applications, can be pursued in a coherent, forward-thinking manner.

Collaborative projects could be managed in several different ways depending on the size and time-scale of the project and number of participants. Two basic management models could be:

1. Public sector researchers to begin projects at universities or associated institutes, which are then moved to the European Materials Science and Technology Centres and further developed with industrial scientists for application or sale to industry.

2. Industrial researchers to work with public sector scientists at materials research centres during all stages of development, under the supervision of one of the centre's group leaders.

Both types of research centres (Materials Science and Materials Technology) should receive direct funding from the European Commission, but public sector scientists should also be allowed to perform research for private companies on a contractual, fee-paying basis. Intellectual property issues such as the right to publish results or maintain company secrecy and so on would have to be clearly set out at the start of each project. These needs present no major obstacle to such research being performed successfully.

8.6.3. European Centres of Excellence (ECE)

The title of "European Centre of Excellence" (ECE) should be awarded to a limited number of materials science institutes to distinguish them from the Centres of Competence in recognition of a sustained world-class level of performance. Strict and impartial selection criteria would be needed that are based on scientific excellence, peer review and recognised achievement. These criteria should be developed and agreed upon by the European Materials Science Board. Candidate institutes should be chosen from the Centres of Competence in Materials Science and Technology described in Sect. 8.6.2.

European Centres of Excellence should be given increased funding to attract the best research staff and pursue large-scale research projects. The mandates of these centres should be to perform materials research that will be of benefit to Europe and Europeans. The awarding of ECEs could by way of example be conducted every 5 years.

(a) Selection and review procedure

To ensure that the title of ECE corresponds to the highest level of expertise in materials science, strict selection and review criteria should be formulated by the European Materials Science Board.

(b) Role of ECEs in materials science in Europe

As well as performing long-term, large-scale research projects at the forefront of materials science, Centres of Excellence should also:

- coordinate European Commission research programmes in materials science;
- form a *European Materials Science Board* to advise on materials research policies and guide their implementation;

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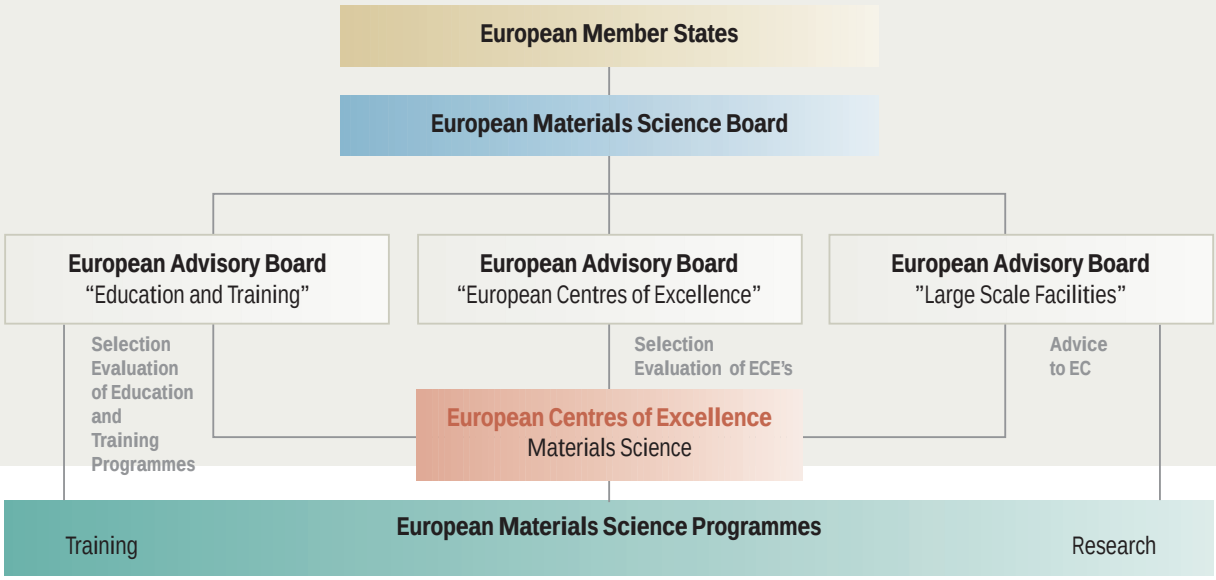

Fig. 8.5. Proposed advisory scheme for European Centres of Excellence in Materials Science.

- act as a think-tank in materials science to seek new research directions;
- organise training programmes in conjunction with industry, providing qualifications recognised throughout the EC;
- organise and sponsor public relation activities (news reports, TV programmes, science fairs and Open Days).

(c) Infrastructure of ECE

To remain at the forefront of scientific excellence, ECE will need:

- Long-term support for the research programmes and missions listed under b).
- Top salaries to ensure competition for places and high quality applicants. Being awarded a position at an ECE should be seen as a mark of distinction.
- Installation of an efficient management office for European Materials Science
- An annual budget sufficient for maintaining and upgrading equipment and facilities.

The proposed advisory scheme for ECEs is shown in Fig. 8.5. ECEs should aim to be the best in the world in their particular field, attracting the world's best scientists and fostering a culture of continuous innovation and openness to new ideas. In their advisory role to governments and the EC, ECEs should seek the advancement of materials science research for the benefit of European society.

8.6.4. Virtual Research Centres ("European Networks")

Materials research has advanced to a point where it is often impractical and sometimes impossible to assemble in one place all of the intellectual resources and specialised equipment for a given research project. Progress in this field depends on establishing effective partnerships across disciplines and among universities, research institutes and industry. This networking enables cross-disciplinary research, leveraging of resources with optimum use of infrastructure and facilities, and provides awareness of the latest technology and potential industrial applications. In addition, it shares the risks and returns of long-term research and assembles teams that can emulate the fertile research environments of large research laboratories.

The seeds of European networks lie in the active, but sometimes small-scale, scientific networks that already exist between universities, research institutes and industry. The European Commission should provide further incentives for the formation of partnerships between groups with complementary skills in appropriate subfields of materials science. The EC should make resources available through special programmes that stimulate European networking. The EC Thematic Networks and Marie Curie scholarships are excellent first initiatives and a good base for further development.

An attractive alternative to establishing "brick-and-mortar" Centres of Competence is for the EC to fund "virtual" materials research centres in the form of networks of four to ten pre-existing materials research labs and institutes. These could consist of groups from academia, public and private research institutes and industry.

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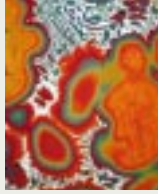

8.7. New Strategies for European Research/ Projects and Project Management

The success of several institutes in Europe with their many technological spin-offs over the past half century, stems from their ability to:

- integrate long-term and expensive fundamental research programmes with training of postdocs and students,
- establish multidisciplinary teams of experimentalists and theoreticians,
- keep in mind the possible applications that new discoveries could engender.

The development of the European Research Area (ERA) should seek to provide similarly favourable conditions for research to institutions throughout Europe, including Centres of Competence in Materials Science and Technology. Management structures for large, long-term research projects should be set in place that are flexible and non-hierarchical. Bureaucracy should be minimised with a simple application process for EC funds (at least for the initial stages of proposal), and the money awarded as a grant, rather than on a contract basis, delegating responsibility of how funds are spent on the principal institutes and researchers. The EC should pass on much of the administration of the projects to national and local research authorities under the supervision of the European Materials Science Board.

Several large scale, multidisciplinary projects will be needed, if Europe is to compete with the economic powerhouses of Japan and the U.S. in materials science and technology. Such projects should be organized as soon as possible for the following priority research areas:

- Nanomaterials
- Surface science (incl. catalysis)
- Smart materials
- Biomaterials
- Materials for alternative energy sources
- Materials modelling

To ensure that long-term materials research is pursued in a sustainable way, experts in basic science need to be included in joint European Research Councils and their recommendations passed on to industry, governments and the general public. Major industrial companies have close links with national governments and the EC, and their views are well represented. Similar lobbies for materials science in academia, as a result of lack of organisation and a unified voice, are less influential. In order to avoid short-term goals taking priority over the long-term research projects needed for fundamental breakthroughs, it is therefore important for scientists in the public sector, particularly those from universities, to take on a more advisory role in national science programmes and the EC Framework Programmes.

A new long-term commitment to research in fundamental science is needed in Europe. Most fundamental research programmes in new areas do not start producing commercially useful results until after several years, so plans for basic research should extend beyond the five-year period of each Framework Programme to ensure that investments of time, brainpower and taxpayers' money are not wasted. As recognised by the research community in Europe, many of these highly interdisciplinary projects are beyond the means of individual institutes, companies or even some Member States. It is therefore strategically important for Europe to promote inter- and transdisciplinary research in the manner described in Sect. 8.4 and elsewhere in this document.

The new Materials Science and Technology Centres should be given as much autonomy as possible, while still maintaining a transparent management structure and being subject to external assessments by acknowledged experts in the field. Fundamental research programmes should not be managed by administrative bodies but by research team leaders who should retain financial accountability and be allowed to develop their own research styles. Researchers, technicians and engineers need to work closely together to complete projects.

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8.8. Relations between Academia and Industry

A recent trend throughout Europe has been for the private sector to take a much more active role in setting the research priorities and goals of university materials science departments. Today's universities therefore often find themselves pulled in many different, sometimes contradictory, directions. One of the hazards of commercialising research at the university level is that the free flow of ideas and information can be hampered as scientists and financiers seek to protect their investments and gain advantages over their competitors. There can also be serious conflicts of interest when researchers' expectations of financial reward bias the interpretation, reporting or selection of experimental results. There is therefore a pressing need to untangle universities' relations with industry, and clarify both their roles in wealth creation.

Allowing scientists at universities to pursue curiosity-driven research free from commercial constraints is the only way to ensure a truly innovative research environment. In the long term private industry and the European economy will benefit from the new ideas and discoveries that will be made. For example, many of the materials breakthroughs made in U.S. industrial labs last century occurred when scientists were given budgets and freedom to pursue their own ideas, rather than following a fixed corporate strategic plan. The European Centres for Materials Science and Technology proposed in Sect. 8.6 could fill some of this need by moving the commercialisation aspects of fundamental research beyond the university environment, while still maintaining close ties between university labs, public institutes and industrial labs.

While outsourcing of basic research to universities by the private sector offers substantial benefits to both sides, it is also important that industry be encouraged to establish and support their own in-house research labs. Without sufficient investment in its own basic research, the innovations necessary for the continued growth and competitiveness of a company are less likely to be forthcoming, as university departments cannot apply as concentrated an effort to a practical problem as the company itself can. The EC and individual governments should therefore take rapid steps to encourage businesses to invest more in research, both basic and applied, short-term and long-term, at universities and their own laboratories. Each country that does this is making a wise investment in its own future.

These suggestions are made with the aim of balancing industrial research needs with the need for “blue skies” research and teaching at universities to maintain the highest standards of academic excellence. The issues are extremely complex, and a great deal more discussion needs to be carried out between all parties involved.

8.9. International Collaboration

European Centres for Materials Science and Technology, along with other university departments, government and industrial laboratories, should establish and maintain strong links with non-European institutes where world-class research is being performed, for example in North America, Australia and the Far East. These links should be chosen judicially on the basis of similar research goals and/or complementary skills/equipment. Competition between different laboratories both within Europe and around the globe can also motivate researchers to work harder and pursue innovative lines of thought.

International exchanges via fellowship programmes with the EC should be expanded. Exchanges and collaborative arrangements should also be encouraged with countries such as Russia, China, India and Mexico, with their large pool of talented, but under-resourced, scientists. To encourage more researchers to spend time working in other countries, greater support for language training and relocation costs should be given, including help in finding jobs for spouses and schools for children. International research projects in materials science should also be broadened through collaboration agreements at the government level. These projects should be accompanied by improved communications channels, e.g., video-conferencing capa-

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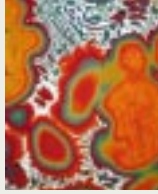

bilities, and provide frequent opportunities for researchers from the different countries to meet and discuss their results, e.g., at conferences and workshops. Opportunities for participating in international research projects should also be more widely advertised and brought to the attention of as many European researchers and laboratory directors as possible.

Science is an international activity that benefits from and even depends on the sharing of ideas and techniques from diverse individuals, countries, and cultures. Major scientific breakthroughs can only be achieved through international collaboration.

Annex 1 – A European Network of Excellence in Catalysis

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An efficient way to enable the European chemical industry to become more competitive on a global scale would be the creation of a Network of Excellence in catalysis, known as the European Virtual Institute for Catalysis (EVIC). Its sole task should be to generate a technology platform that enables the chemical industry to better develop improved and new processes. It should bridge the gap between knowledge-driven fundamental science and application-driven R&D. Academic research develops methods of investigation and concepts of catalysis remote from practical problems and at a level of understanding which cannot simply be extrapolated to practical catalysis. Industrial R&D, on the other hand, operates on a more empirical basis and does not have the focus nor the resources to build a comprehensive theoretical framework.

This Network of Excellence should bridge the gap between these two streams of activities. It should operate at the highest level of scientific excellence and seek to solve problems fundamental to all industry and not just a specific company. The results from EVIC should enable individual companies either internally or with bilateral research agreements with one partner from the network to develop company-specific technology. EVIC should be interdisciplinary with a structure similar to the general outline sketched in Fig. A1. The network proposed here should work on all types of heterogeneous, homogeneous and biological catalysts.

In order to remain independent of individual company interests EVIC should be financed completely from European Commission resources. A range of potentially inter-

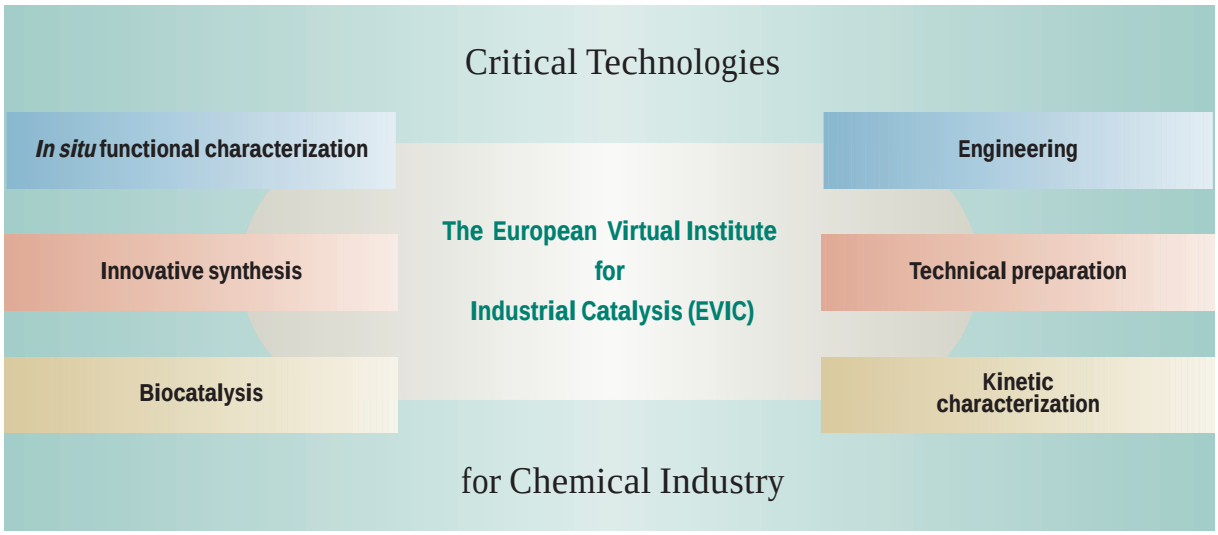

Fig. A1. Outline of EVIC as an interdisciplinary technology platform enabling improved chemical process design.

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ested beneficiaries is given in Fig. A2. Participation in the network should be kept open to all parties interested at any time, even also after its foundation.

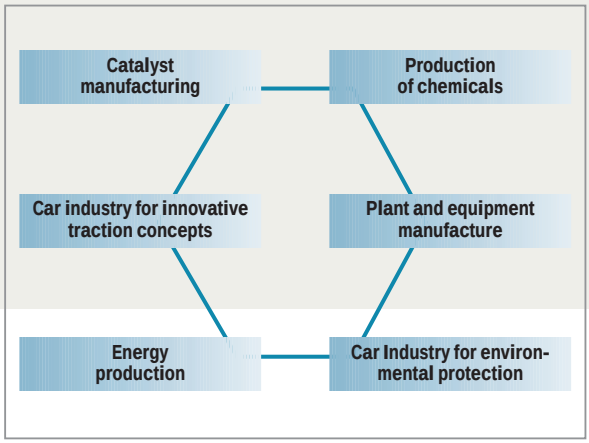

Fig. A2. Industrial sectors that could benefit from EVIC. The fundamental and strategic character of catalysis becomes clear from the range of businesses concerned.

The research projects should be decided by the industrial partners to ensure that all activities are application focussed. Project leaders should be established scientists in order to ensure the highest scientific standards. This arrangement is only possible with a virtual structure that allows leaders to remain in their normal working environment. A number of administrative and coordinating officers working full-time will be needed to support the project leaders. Fig. A3 illustrates the organisation of such a network. A small nucleus of full-time staff supports the part-time researchers and project leaders by coordinating project operation with multi-national consortia.

EVIC will require independent funding and a time schedule suitable for the problem. Four periods of three years should be suitable for most long-term projects, with initial and four intermediate international audits. The auditing commission should be led by the beneficiaries (see Fig. A2) supported by academic experts from around the world. In this way the network can be run independently of short-term economic constraints and is guaranteed not to lose its focus on the pre-commercial R&D.

The network should have six departments and be led by a council of the six departmental heads. The six departments proposed are shown in Fig. A4.

EVIC should bring together the best European researchers for a given task. Participation should be granted strictly upon scientific excellence in the required field and on no other criteria. Europe has competent scientists in all areas shown in Fig. A5. However, substantial and reliable funding is needed for collaborative research within a timetable sufficient for an in-depth research effort uninterrupted by fluctuations in short-term funding.

EVIC should support medium- (6 years) to long-term (12 years) research into generic aspects of catalysis in the fields mentioned above. This research must be application-driven and should not be curiosity-driven. Studies aiming at fundamental understanding of complex technical processes using validated models under relevant conditions should be part of the research profile of EVIC. Experimental studies on model catalysts under remote operation conditions and purely synthetic projects are too academic and should not be part of the activities of the Centre. Development of rational synthesis protocols for

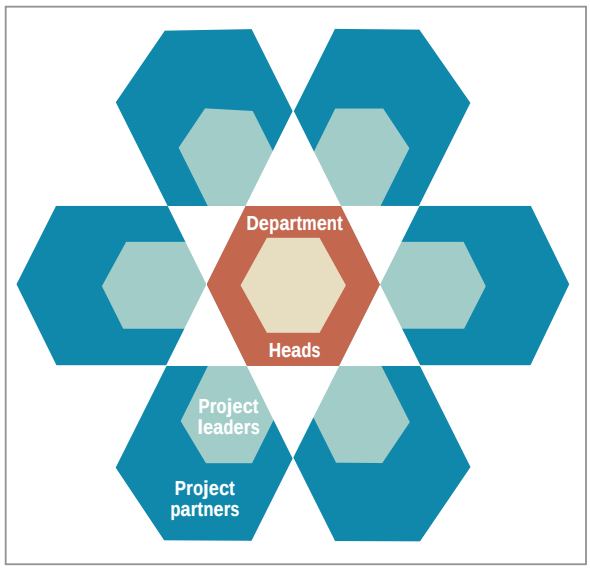

Fig. A3. Schematic representation of the organization of a network of excellence.

existing catalysts and search strategies to identify novel materials for catalytic applications (combinatorial chemistry) including the development of supporting technologies may, however, be a task of EVIC. The broader application and methodical developments of *in situ* characterization with the aims of integrating large-scale facilities (synchrotrons, neutron sources) and also providing cell designs and attachments to commercial laboratory instrumentation should be another task. The development of theoretical concepts at the *ab initio* level as well as the broadening of microkinetic analysis as research tools may be further tasks.

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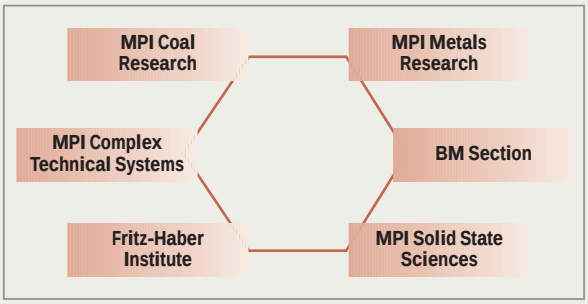

Fig. A4. Centres of competence within the Max Planck Society that could contribute to EVIC. Their long-term commitment would make them ideal as integrators for other activities being pursued in Europe.

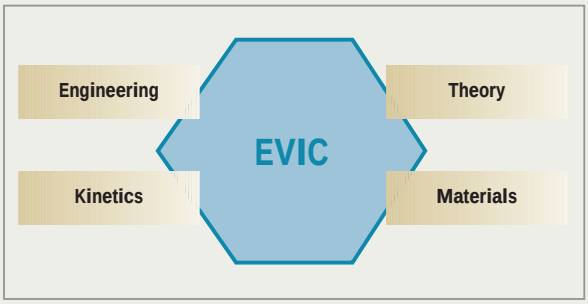

Fig. A5. Strong interaction between the departments is necessary to ensure that the most is made of the interdisciplinary nature of EVIC if innovative catalysis research is to be performed.

Particular emphasis should be placed on the broader application of biotechnology in catalysis. The discrepancy between the potential of this technology and its representation in current industrial practice is striking and may be caused by a lack of proof of operability and of economic feasibility in other than highly specialized drug synthesis processes. Development efforts and piloting processes, as well as solutions to problems concerning the compatibility of biological catalysts with conventional chemical environments, may be special process-specific goals.

The output of all projects should be continuously monitored by auditing assessments and reports to industrial working parties about the activities of EVIC's six departments. The projects should be selected via a bottom-up process with participation of industrial partners who provide guidance and are willing to test the results of the projects within their own research but without active financial contributions. Intellectual property rights should be guaranteed to the industrial partners while also protecting the rights of the academic partners.

Each of the six areas of activity mentioned above should be conducted by groups of several consortium members. A nucleus of institutions committed long-term to EVIC should seek to persuade existing projects in Europe (e.g., national virtual catalysis projects) to coordinate their activities with those of EVIC. For example, Fig. A4 shows the different partners of the Max Planck Society which have interest or skills in catalysis technology.

Internationally known virtual centres such as NIOK in the Netherlands, CONNECAT in Germany, or institutional centres like in Strasbourg (ECPM) and Lyon (IFP) and the British Leverhulme Centre for Innovative Catalysis, should contribute to the nucleus of institutions supporting EVIC.

EVIC's finances should be sufficient to cover all costs of travel for researchers, as well as consumables and large-scale equipment. It is important that all projects be conducted with optimum efficiency, in other words, EVIC should maintain state-of-the-art apparatus and instrumentation. The bulk of EVIC's finances should come from contributions from the consortium members. Standard catalytic infrastructure and leading/support personnel should be brought into each project by the participating companies.

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9. Materials Science and Basic Research in Europe: Conclusions and Recommendations

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This White Book reflects the vision of a diverse group of leading scientists in Europe concerning the future of materials science. Experts in the field are convinced that high-performance materials are the basis for all key technologies and, thus, the future of every modern society. There is also common agreement that the challenges concerning the increased complexity of high-tech materials and greater world-wide competition can only be met by well-organized, joint European Commission (EC) research programmes in basic materials science that ensure sustained financial support and the highest level of expertise. A number of recommendations for the European Commission authorities currently preparing the next Framework Programme have been formulated with the sole purpose of making this vision a reality. These recommendations are:

- Materials research in the EC should be given the same priority as biotechnology and informatics. Materials science plays a crucial role in the development and competitiveness of these and many other technologies, especially in the transport, chemical, energy, electronics, and aeronautical industries.
- The EC budget for basic science needs to be increased to a level comparable with that of Japan in order to remain competitive in the 21st Century, in particular with the Pacific region.
- European materials research programmes have to be coordinated to avoid unnecessary duplication between research groups in different Member States, to promote efficient use of resources, and to look for possible synergies.
- The basic research, development and evaluation of materials should fall under the jurisdiction of a European materials science agency, modelled on the National Science Foundation (NSF) in the U.S. or the Swiss Science Agency, with the minimum amount of bureaucracy.
- The EC materials programme should span materials research and materials technology, with emphasis on long-term fundamental research.
- The fragmented nature of materials research in Europe needs to be replaced with a more efficient organizational structure. This could be achieved by establishing Centres of Excellence in Materials Science and Technology to coordinate European-wide research efforts.
- The number of interdisciplinary projects and education programmes has to be increased and greater interdisciplinary networking actively promoted in Europe.
- The EC should investigate plans for ensuring greater researcher mobility to make the most of Europe's diverse skill base and cultural heterogeneity for spawning new ideas. This should include the creation of a professional qualification for materials scientists and engineers (EurMat) that is recognized throughout Europe.
- The EC should commence dialogue with non-scientists and other interest groups to find ways of countering the decreasing popularity of science in society. Steps should be taken to increase the profile of materials science through better education, science fairs, institute open days, summer schools, etc.
- Greater numbers of students enrolling in materials science and related courses at university are needed. This may be achieved by promoting greater awareness of the range of careers available, and also increasing salaries of academics working in these fields.

◀ Transmission light micrograph of a shell obtained with polarized illumination (U. Täffner, MPI für Metallforschung Stuttgart).

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Priority research areas for European materials research should be:

Materials discovery and design

To accelerate the design and exploration of new materials and novel phenomena and properties, priority should be given to the study of improved synthesis and processing, materials theory/modelling and advanced analytical techniques.

Interdisciplinary research strategies

Completely new materials architectures and properties can be expected from the interplay between different types of materials systems, in particular from the design of devices made from inorganic and organic materials on the nano-scale. Interdisciplinary research between physicists, chemists and biologists should be supported and coordinated on a European level.

Special materials with high innovation potential

Smart materials, biomaterials and nanomaterials will be among the fastest growing areas of materials science over the next few decades, as will be materials for alternative energy sources, including high temperature and magnetic materials. Priority should also be given to materials that improve our management of the environment, natural resources and recycling. Such areas should become an important part of the EC's long term research plans and suitable funding should be made available to ensure Europe leads the way in each of them.

This White Book should be regularly updated to serve as a source of ideas for policy makers, and academic and industrial research directors. In the following sections, key aspects regarding the future of materials science, including technological trends and research priorities, are summarized and recommendations made. With a concerted effort from all European researchers, institutes and governments, Europe can succeed at the forefront of materials technology and enhance both her economic performance and the standards of living of her citizens.

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9.1. Materials Phenomena and Techniques

9.1.1. Materials Phenomena and Properties

Understanding, control and tailoring materials phenomena and properties on a microscopic level are key targets in materials science. By doing so we can develop new materials to meet technological needs, and optimize materials use to reduce wastage and pollution.

In the past, the primary task of materials scientists was to quantitatively characterize phenomena and develop modern theories to explain them. Today we have accumulated detailed knowledge of a large number of different electric, magnetic, optical, mechanical, and thermal phenomena described in terms of classical or quantum correlations in condensed matter (Fig. 9.1). Materials science beyond the year 2050 will be characterized by the control of materials phenomena on the nanometre length and femtosecond time scales. Several major targets exist for future analytical techniques, such as:

Microstructural design: The further improvement of our understanding and control of mechanical, thermal and chemical properties of multicomponent alloys, composite materials, materials with nano-sized components, and ceramics is needed in various key technologies. A major challenge here is the multiscale nature of many phenomena, which requires detailed understanding of how structures at different length scales interact and influence each other over different time scales. This will require considerable effort on various fronts, including modelling and microscopic analysis.

The tailoring of phenomena in a controlled and reproducible way using nanotechnological concepts: Since most materials phenomena are of a cooperative nature, they depend strongly upon the size of the system and are effected by the presence of surfaces and interfaces. This will allow tomorrow's materials scientists to modify, for example, the electric and magnetic response of artificial structures to the precise values desired. Materials science is an extremely diverse and multidisciplinary field that covers a wide range of novel phenomena, often with the potential for immediate applications.

Small-scale phenomena: The small-scale regime offers real opportunities for developing sustainable and environmentally friendly materials that meet tomorrow's technological needs. Colloidal systems and biomimetic strategies are two examples of an array of new concepts that will allow us to design small-scale systems with greater multifunctionality. The size dependence of properties such as hardness and superplasticity will give rise to new mechanical phenomena ("smaller is tougher") and new thermodynamic behaviour that will have enormous impact on future technologies.

Dynamic response of systems over very short time scales: Understanding and (in future) controlling ultra-fast processes in materials is currently of great scientific and technological interest. It has recently become possible to probe dynamical phenomena in materials on ultra-short time scales down to sub-picoseconds (see Sect. 9.4). The study of ultra-fast structural relaxation phenomena will improve our understanding of phase transformations and structure formation. Rapid switching of magnetic domains in artificial structures will be used in tomorrow's information technology. These are just two examples of this important emerging field. Strong input and guidance from materials analysis and materials modelling will also be indispensable.

The study of phenomena under extreme conditions: The behaviour of materials under high pressures, high temperatures, high magnetic and electric fields is still poorly understood. Such studies are complicated and require expensive and sophisticated instrumentation, but have become possible with the availability of equipment for producing extreme external fields.

Dynamic and dissipative phenomena at surfaces and interfaces: With further developments in nanotechnology, the need to understand dissipative phenomena, lubrication and friction on an atomic level and in systems confined to the nano-scale will increase rapidly. These studies will ultimately lead to *in situ* studies of atomic friction on ultra-short time scales. Microscopic insight into the structural changes that take place during corrosion and catalytic and electrolytic reactions are of fundamental importance for the active control of these chemical reactions, in which both molecular reactivity and surface morphology play a role. It has become clear during the last few years that the ultimate understanding of these (also technologically important) physicochemical phenomena requires microscopic information of the dynamic behaviour of both electrons and nuclei. This information can only be obtained using spectroscopy-microscopy and spectroscopy-diffraction techniques in real time (see Sect. 9.1.4).

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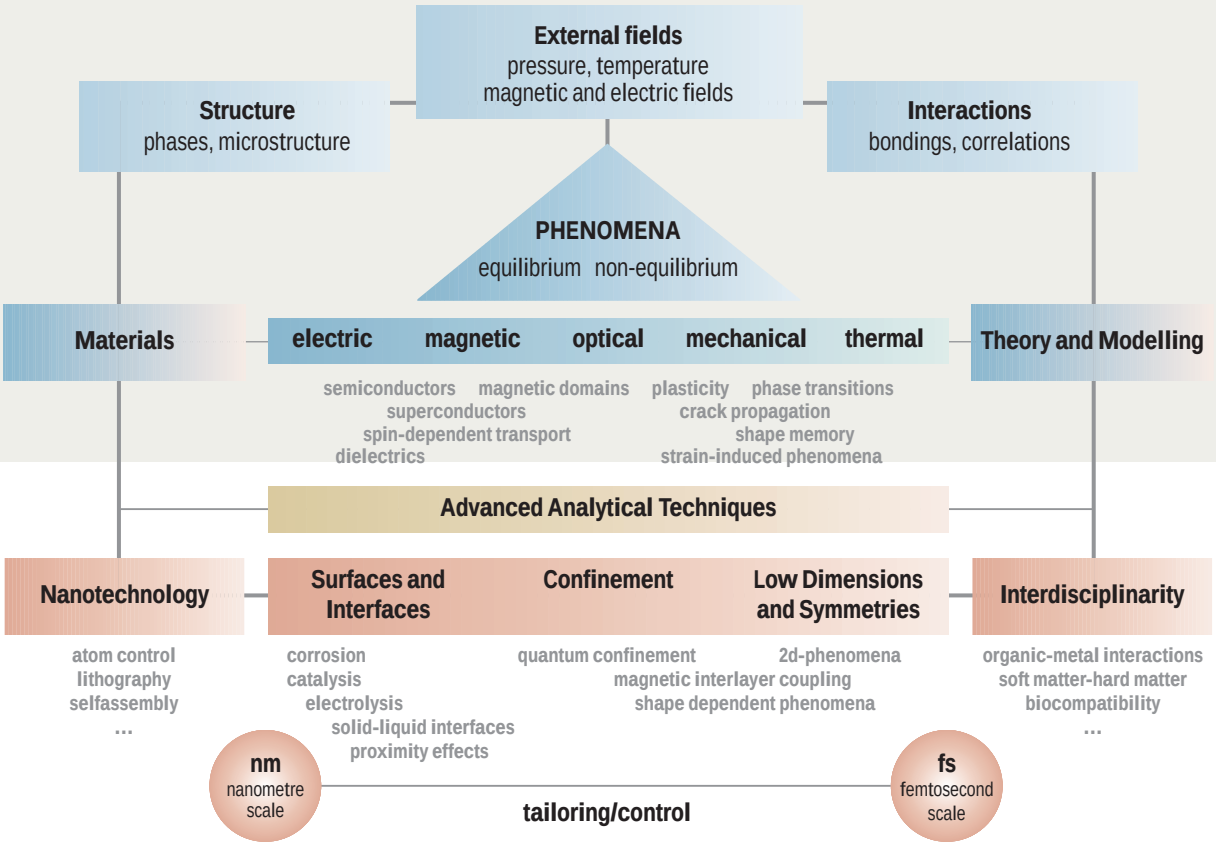

Fig. 9.1. Materials phenomena: interrelation between materials, modelling, analysis and future trends.

9.1.2. Synthesis and Processing

Synthesis and processing are fundamental to materials R&D, with new or improved methods usually leading to new materials or superior properties. Synthesis and processing are also responsible for the production of high quality, low cost products throughout the manufacturing industry. The main areas of innovation in synthesis and processing are:

- increased control over complexity, composition, structure, and function;
- water-based solution chemistry for low-cost, environmentally benign synthesis;
- rapid forming for use in combinational chemistry and the search for new materials;
- tailoring of materials at all length scales, from the atomic to macro-scales;
- computer modelling of complex phenomena to improve understanding and control;
- thin films and coatings for improved properties and component lifetimes;
- supercritical fluid chemistry for preparing new materials and nanomaterials as oxides, nitrides, metals with controlled both shape and size, continuously from micronic to nano-scales.

Basic research is still needed in the areas of crystal growth, vapor deposition, sintering, phase transformation, and rheology to better understand how they affect and can be controlled during synthesis and processing. Fig. 9.2 outlines the main areas of development for these techniques in the future.

Recommendations for priority research areas in materials synthesis and processing are:

Miniaturization

Miniaturization will be one of the most important goals of materials synthesis and processing in the near future. New processing technologies will be required to create all kinds of materials on ever smaller length scales. These techniques will enable manipulation of individual nanostructured units and atoms, and should be amenable to auto-

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mation and parallel processing so that combinatorial approaches can be used to discover and optimize materials.

Biomimetics and biomaterials

The field of biomimetics is one of the most challenging fields for synthesis and processing of organic materials. In medicine, new biomaterials are urgently needed for a variety of uses (e.g., implants, biosensors). It is still not clear, however, how such materials can be synthesized in a well-controlled and reliable fashion, since the knowledge on biomineralization and other natural synthesis processes is still in its infancy.

Complex structures with building blocks/assemblies

Complex, functional structures or assemblies are constructed from building blocks on both the nano- and the meso-scales. Structure development is driven by self-organization. The confinement of highly dispersed Nano Building Blocks (NBBs) in hybrid or inorganic matrices or the organization of NBBs on textured substrates could provide larger concentrations of active dots, better defined systems, avoid coalescence into larger ill-defined agregates while keeping or enhancing specific magnetic, optical, electrochemical, chemical and catalytic properties into the nanostructured hybrid materials.

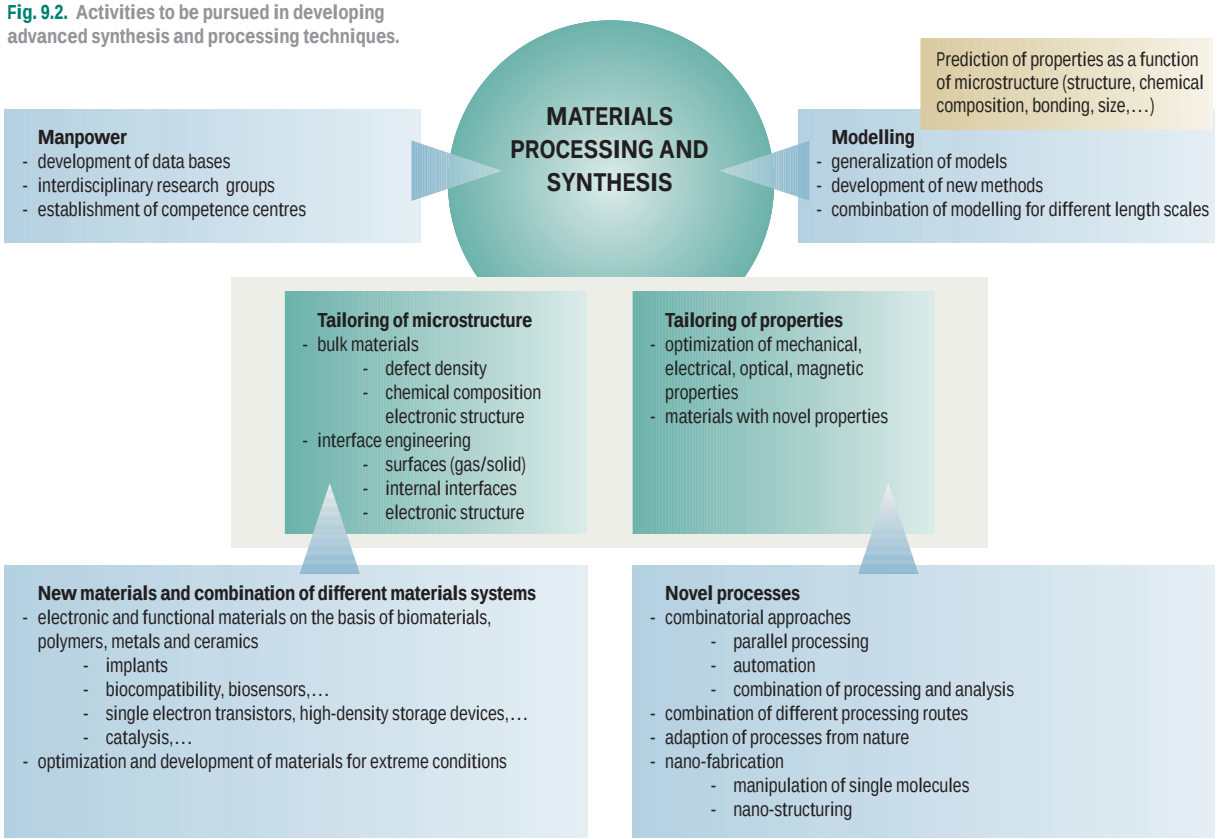
Interface engineering

Interface engineering is an increasingly important means of improving and optimizing all kinds of materials from metals, ceramics and superconductors to bio- and smart materials. This field includes processing and tailoring of surfaces and interfaces for special applications like microelectronics and catalysis. Miniaturization results in interfaces becoming one of the dominant defects in a material; in some cases, these interfaces are necessary to obtain specific phenomena. Interface engineering is therefore a vital component of many future technologies.

Modelling and automation of materials synthesis and processing

Trial-and-error experimental approaches are inefficient ways of designing and discovering materials. Modelling of synthesis and processing is a powerful tool for deciding which directions to pursue, and which are non-feasible or uneconomic. These techniques have proven valuable for many years in traditional fields, like steel processing. Although urgently needed, modelling of nano- and biomaterials processing has only just begun. Automated processing must be sufficiently accurate if it is to be used for nano-fabrication.

Fig. 9.2. Activities to be pursued in developing advanced synthesis and processing techniques.



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9.1.3. Advanced Analytical Techniques

Progress in materials science is intimately related to achievements in the development of dedicated analytical techniques which enable us to examine the atomic and electronic structure of materials on the nanometre level and to unravel and quantitatively analyze condensed matter phenomena and processes. The current and future roles of modern techniques in the analysis of materials are summarized in Fig. 9.3.

Future targets in the design and processing of new materials, and monitoring and control of new phenomena and properties, are the generic driving forces for the development of new concepts and new techniques in diffraction, microscopy and spectroscopy. The highest possible resolutions, greatest sensitivities, and ultimate detection limits are the chief goals of this field, along with performing non-destructive and in situ analysis. One consequence of developments in this area will be that the traditional boundaries between the three major analytical methods (diffraction, microscopy, spectroscopy) will gradually disappear.

One possible scenario for how this key field of materials science can be organized in Europe is shown in Fig. 9.4. The following challenges in advanced analytical techniques will need to be met in the next decades:

High resolution microscopy

To obtain local, non-averaged structural information about inhomogeneous materials and structures, improved instrument resolutions will be needed to access smaller spatial domains, e.g.,

- sub-Å and sub-eV resolution in high resolution electron microscopy,
- 10 nm spatial resolution in X-ray microscopy.

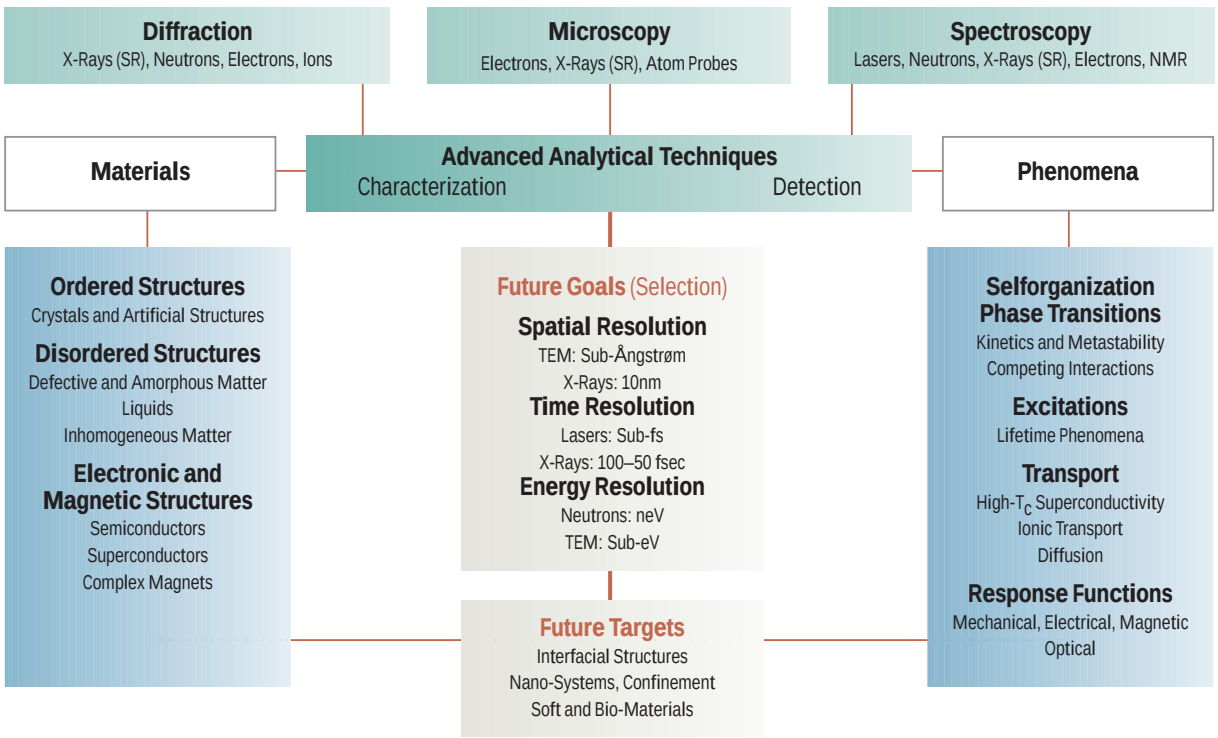
Real time characterization of materials and phenomena on femtosecond time-scales

The ultimate goal of this endeavour is to observe atomic motion in materials, particularly during chemical reactions and biological processes, directly. The same techniques could be used to control short-time relaxations of electrons and atoms during materials processing (e.g., modifying materials by ion beams). Quantifiable objectives include:

- 1 fs time resolution in laser spectroscopy
- 10 fs time resolution in X-ray diffraction

Achieving these ambitious goals, and thereby providing revolutionary insights into materials, will require new and expensive equipment and facilities, e.g., free-electron X-ray lasers. Such large-scale facilities can only be built and operated on a European level with strong commitment from Member States.

Fig. 9.3. The role of advanced analytical techniques for materials science, including future goals and targets.



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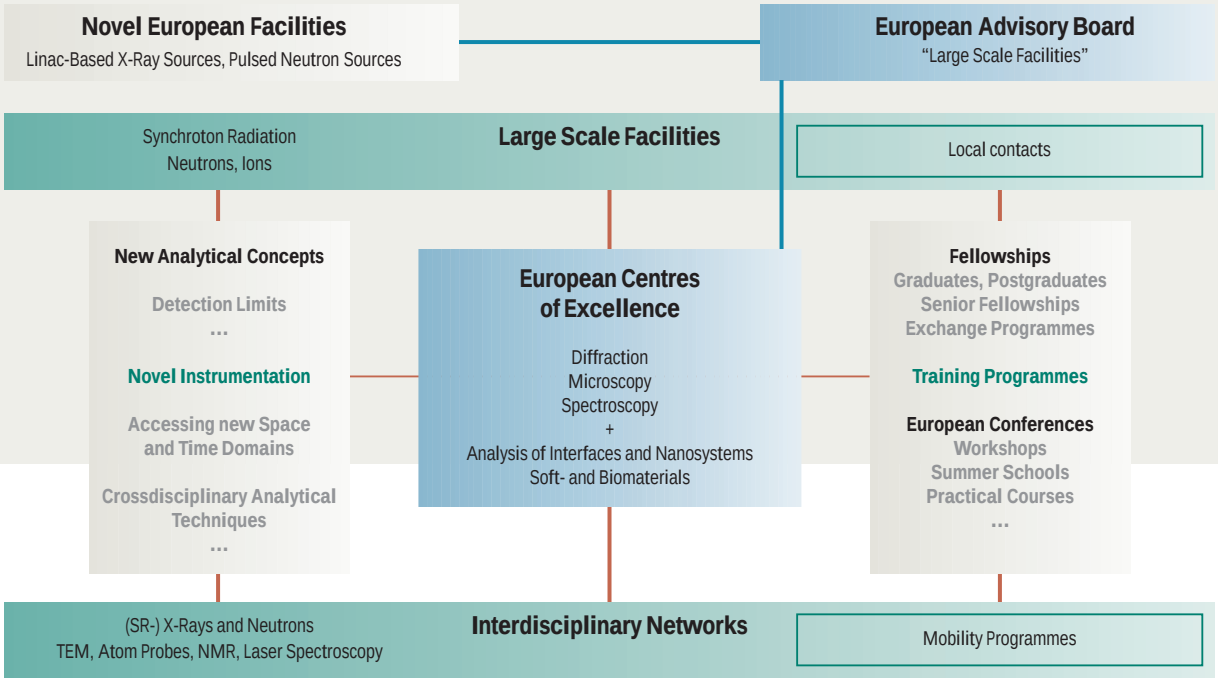

Fig. 9.4. European action plan for advanced analytical techniques.

Efficient use of European large-scale facilities and modern techniques in materials analysis

New concepts in analysis are often developed by solid state physicists in dedicated laboratories or large-scale facilities with little or no contact with the materials scientists who could apply new techniques to the solution of "real world" problems. The efficient transfer of new ideas and breakthroughs in diffraction, microscopy and spectroscopy to the materials science community needs to be promoted by holding cross-disciplinary workshops and training courses. The institutes housing state-of-the-art facilities should also provide professional assistance to outside parties and act as "local contacts" with developers of new techniques.

Creation of analytical networks and centres of excellence

The full potential of current and future analytical methods and apparatus can best be exploited if networks and centres of excellence are created which manage world-class facilities and provide high quality research and training opportunities.

9.1.4. Materials Theory and Modelling

Computational materials science and engineering provide powerful tools for:

- prediction of novel structural and functional materials, e.g., nanomaterials,
- optimization of complex materials/design solutions
- simulation of materials synthesis, processing, microstructures and properties,
- development of history-dependent and of scale-bridging multi-scale simulation concepts,
- integration of electronic and atomic level as well as continuum scale approaches,
- studying phenomena that are not easily accessible by experiment,
- solving cost and time constraints for materials development and application.

A large number of computer modelling techniques are available for studying all kinds of materials and their behaviour from the quantum and atomic levels to microstructural and macroscopic levels over various time spans. Materials modelling will play an increasingly important role in materials design and the understanding of both fundamental and complex processes in all materials. The major themes for materials theory and materials modelling to be pursued within the EC over the next ten years are summarized in Fig. 9.5.

The following recommendations are made for ensuring Europe remains at the forefront of computational modelling of materials:

- Supercomputer facilities need to be installed or upgraded at more sites for large-scale simulations of fundamental materials processes and phenomena, e.g., sintering, crack propagation, catalysis.

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- Interdisciplinary teams are needed to develop robust software and examine complex phenomena and materials.
- Computer laboratories in materials science departments need to be expanded and upgraded to include the latest PCs, workstations and simulation software tools.
- Training courses in materials modelling should be held regularly throughout Europe for students, academic and industrial researchers
- Networks for materials modelling are needed to aid long-term, large-scale simulation projects.
- Development of multi-scale modelling techniques should be given greater priority. This could be done by organizing collaborative projects between groups specialising in different simulation methods and length/time-scales.
- Collaboration between industry and academia in the development of simultation methods should be promoted.

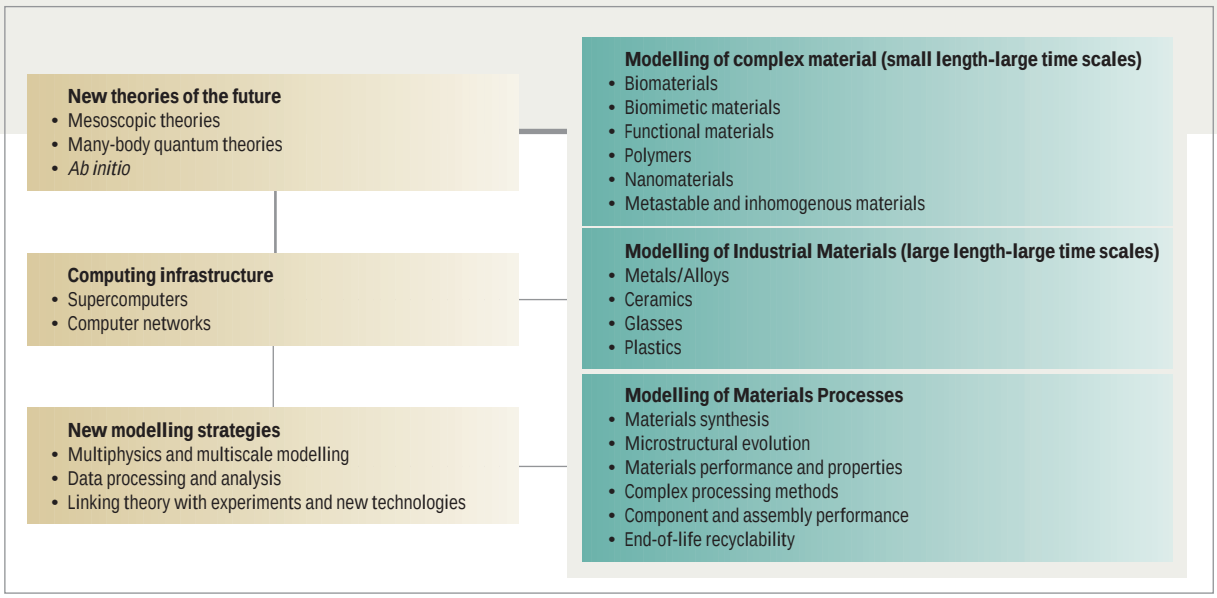

Fig. 9.5. Research priorities for materials modelling over the next decade.

9.2. Materials Systems

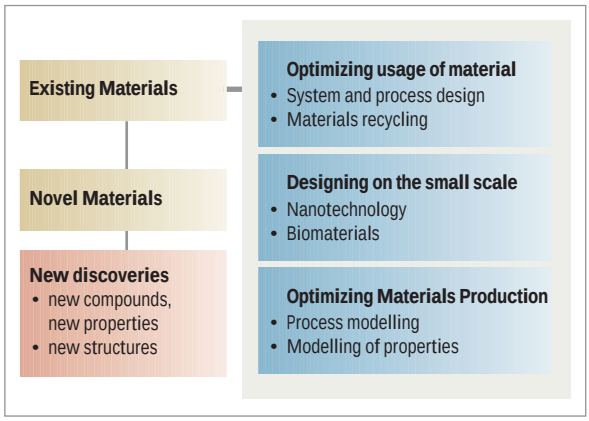

Fig. 9.6. Overall strategies for improvement of advanced materials into the 21st Century.

Materials can be divided into two broad groups; inorganic and organic materials. Inorganic materials are composed of non-carbon-based matter such as metals, ceramics and metalloids (e.g. silicon and germanium). Organic materials are based on carbon compounds, and include both living tissue and synthetic polymers. Materials can also be divided according to their properties or main applications, e.g., semiconductors, nanomaterials and catalytic materials. Technological progress in materials science can be brought about by modifying and improving existing materials or by developing novel materials resulting from new discoveries. These concepts are outlined in Fig. 9.6.

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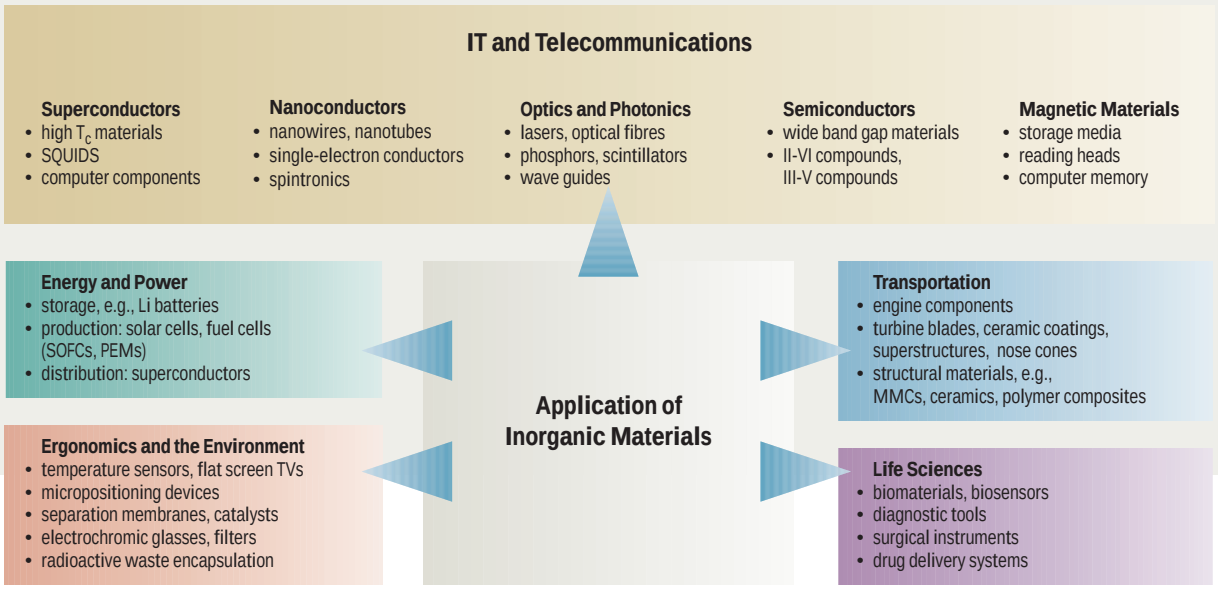

Fig. 9.7. The diversity and range of applications of inorganic materials.

9.2.1. Inorganic Materials

Research into advanced inorganic materials over the next ten years will reap benefits for five important sectors of the economy (Fig. 9.7). In all cases, basic research will be directed towards developing new synthesis methods allowing greater control over structure formation and smaller scale components. Research should also be directed at discovering new materials and compositions, structures and phenomena that will spawn new technologies, and revolutionize the way we manufacture goods, conduct business and spend our leisure time.

(a) Metallic materials

Metals and their alloys have the potential for further large improvements in properties and performance during the 21st Century. Due to their high stiffness, ease of forming, strength over a wide range of temperatures and, most importantly, their reliability, metals are the materials of choice for many engineering applications. They also often serve as the main phase in composites and adaptive systems because of their attractive properties. They range from low-cost bulk materials used in civil engineering to advanced, high added value materials tailored at the atomic level. The need to improve their corrosion resistance and their potential for recycling are important reasons for maintaining a high level of scientific, technical and industrial R&D in this field.

The basic scientific challenges lie particularly in pursuing fundamental and long-term oriented research in this field that is aimed at the development of well-tailored structures. Major challenges lie in the development of lightweight structural materials, self-organizing microstructures, failure-tolerant materials systems and smart materials.

Metallic materials can be divided into four categories according to their present and future impact on economic and industrial activities, as summarized in Fig. 9.8. Important areas of metals research for the future include:

• Microstructural design of structural metals, alloys and their composites

Much remains to be understood concerning the microstructural design and optimization of multiphase metallic materials, which represent a large fraction of engineering structural materials. The corrosion and heat resistance of steels could be improved by better microstructural control, particularly at interfaces. Metal matrix composites also lend themselves to the systematic exploration of variations in multiphase metallic microstructures. Other important objectives include developing high strength-to-weight ratio structural materials, self-organising microstructures, failure-tolerant materials systems and smart materials.

• The physics of plasticity and damage

Better understanding is needed of the complex phenomena involved in deformation and fracture of metals, alloys, and metallic composites. New techniques for modelling the micromechanical behavior of materials that incorporate substructural phenomena (i.e., dislocations, boundaries, interfaces, and microvoids) coupled with focused experimental work should achieve this.

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• Complex metallurgy

Understanding of phase transformations and microstructural development in multicomponent alloys (e.g., superalloys and tool steels) has vastly improved with the advent of computer codes such as Thermocalc: This research needs to be pursued further for (i) improved understanding of the fundamentals of the thermodynamics and kinetics of phase transformations, (ii) improved understanding of microstructure/property relations of each component from the atomic to macro-scales.

• Liquid/solid processes

Many materials processes involve the coexistence of a liquid with a solid, e.g., liquid phase sintering, rheo/thixocasting, and many composite fabrication processes. The physics of such processes have much in common, including the influence of capillarity, and fluid flow in the presence of fine-scaled solids. Progress in understanding and modelling these phenomena would provide significant benefits in terms of reduced costs and higher quality for many materials classes (composites, ceramics, metals).

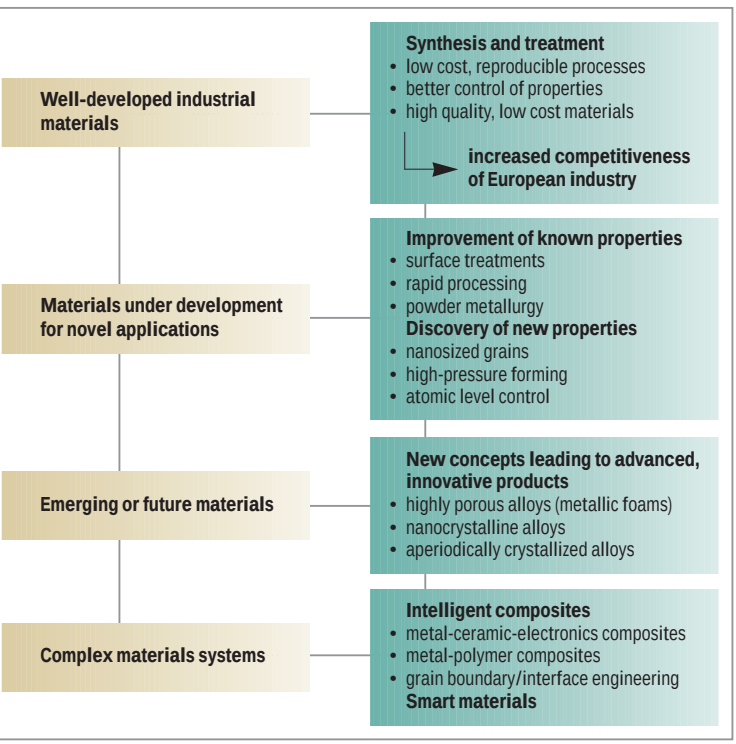

Fig. 9.8. Short-, medium-, and long-term research directions for metallic materials.

• Functionally graded materials

Many structures require materials whose properties vary from one point to another. This leads to the concept of "functionally graded materials" (FGM), which have been the focus of several national research projects in Japan, the U.S. and Germany over the past ten years. Key challenges in this area are to lower the cost of processing, as current FGMs are generally uneconomical.

• Novel metallic materials and systems

Unconventional combinations of different metals, microstructures and properties that have not yet been investigated could yield unexpected and useful materials. Novel synthesis and processing techniques should be used to explore these potential "goldmines". Metals research should become more interdisciplinary, with metallurgists working closer with physicists, engineers, chemists and biologists to come up with new multimaterial systems.

(b) Ceramic materials

A wide range of advanced ceramics are being developed for future applications such as environmental sensors, electronic components, turbine blades and fuel cells. Improved processing and quality control will enable structural ceramics to be used in niche areas such as aeronautics, space flight and power generation. The distinction between structural and functional ceramics will become blurred as smart materials, nanoceramics and bioceramics are developed.

The main directions which ceramics research will take in the future are summarized in Fig. 9.9. New design concepts such as biomimicry, hyper-organization, complex composite architecture and nanotechnology, combined with the increased understanding and predictive power provided by computer modelling, mean that advanced ceramics have a bright future. Challenges and foreseeable trends for ceramics research in Europe include:

Fabricating new architectures via microstructural control and new processing routes. The challenge is to create new classes of materials exhibiting previously unimagined properties by controlling the structure at the nano-level and using low cost and environmentally benign synthesis routes.

Integration of ceramics with other materials. In the future, ceramics will be combined with other conventional materials systems, both inorganic and organic, to provide greater functionality and reliability. These "smart" composites will be used in both structural and functional applications, far beyond the capabilities of most materials currently being used.

Nanotechnology and miniaturization. Investigation and exploitation of effects occurring at the meso- and nano-scales will become increasingly important over the next decade. Decreasing the size of ceramic components and their constituent grains can be expected to reveal a whole range of novel unexpected phenomena that can be put to use (e.g., as sensors or biomaterials).

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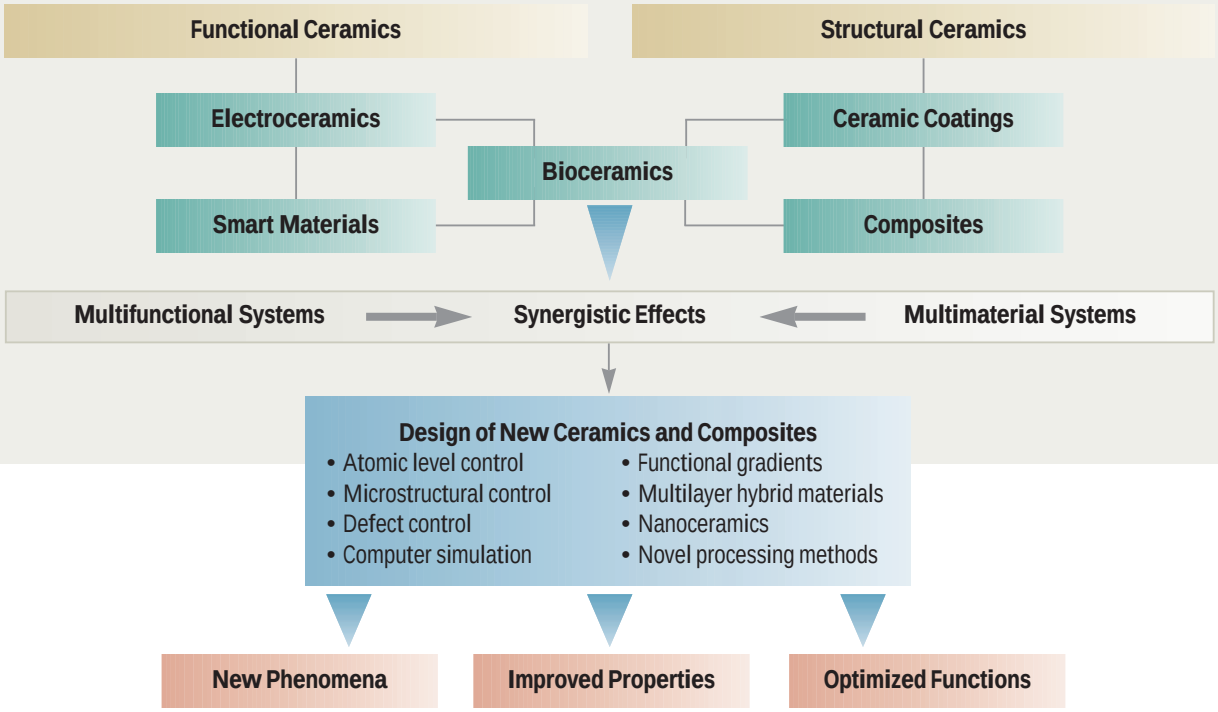

Fig. 9.9. Future advanced ceramics, including design concepts and goals.

Increasing functionality of ceramic materials. A whole range of new compounds and ceramic materials are being discovered with unusual properties that can be used in applications such as electronics, photonics, lasers, recording media, sonar, sensors, displays, batteries, infrared detectors. Intense effort is needed if Europe is to reap the rewards from this rich area of research.

Important recommendations for promoting ceramics research in Europe are:

Greater uptake of advanced ceramics by industry

Industry should be actively encouraged to incorporate the latest advanced ceramics into their products; although initial outlay can be greater, ceramics are generally longer-lasting, lighter weight and more heat-tolerant than alternative materials, so that greater savings are made in the long run. Ceramics also can provide more functionalities than cheaper, high volume materials.

New initiatives in ceramic science

The EC should fund new European-wide initiatives to develop advanced ceramic materials, especially ceramic matrix composites, bio- and electroceramics. Funding should be raised to a level comparable to that in Japan, which currently leads in the development and uptake of ceramic technology. These initiatives should include substantial industrial participation to ensure a critical mass of researchers and availability of the latest equipment in this high-investment, high-returns field.

Establishment of a European ceramics institute

A European institute dedicated to advanced ceramics and covering the whole spectrum of these materials, including interdisciplinary areas such as bioceramics and nanoceramics, would greatly aid uptake of ceramics technology by smaller companies, as well as promote standardization of property measurement, materials quality, and European-wide collaboration.

(c) Amorphous solids - glasses

Long term research into the innovation of new vitreous materials merits special encouragement. This includes the discovery of brand new glass families by the control of subtle interactions among complicated sets of atoms, as well as the mastery of industrial compositions from a chemical bonding point of view. Huge efforts should be made in the understanding of the glass formation mechanisms and the modelling of glass structures.

(d) Structural composite materials

Composites offer the possibility of creating materials with superior properties or improved functionality by combining two or more disparate materials to form a single materials system. The main types of composites currently being investigated include polymer composites, metal matrix

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composites and ceramic matrix composites. In the future we can expect to see an increasing use of biological materials in composites, particularly as research into biomimetic materials takes off and nature's secrets for producing ultra-hard but tough materials from the atomic level are revealed.

The main areas of future composites research should be:

- Smart composites incorporating sensors and actuators,
- Interface studies, particularly of delamination and internal friction;
- Computer modelling of complex architectures and shapes;
- Metal matrix, ceramic matrix and polymer matrix composites engineered on the nano-scale for use in different temperature regimes and exhibiting unique and superior properties;
- Development of new systems, e.g., aluminium-based alloys reinforced with silicon carbide and alumina particles, whiskers or fibres.

One of the greatest challenges for researchers is to understand the many complex interactions between the components of these materials. This requires a systematic approach to understanding, design and production. The creation of a Centre of Excellence for Structural Composites would provide for an integrated multipartner approach to elucidating the fundamentals of processing, design, optimization, and industrial implementation. This would advance the technology significantly and strengthen Europe's position in the field, in which it currently lags significantly behind North America. Transportation, electronic packaging, power transmission, aerospace, and sports technology, to name presently established application areas, would all benefit from improvements in this field.

9.2.2. Organic, Bio- and Biomimetic Materials

(a) Polymeric materials

The field of polymeric materials is broad and extends from basic synthetic chemistry to process engineering. Research has traditionally been pursued in the laboratories of large chemical corporations and chemistry or chemical engineering departments of universities and research institutes. In the last few years a grown interest has emerged in combining knowledge from polymer science and other disciplines. Therefore the potential for creating new and innovative materials is enormous.

Basic research is still needed in many areas of polymer science. Model polymeric materials (low molecular, compositional and structural heterogeneity) are very important in order to understand the basics of structure-properties relationships. Priority research topics in polymer based materials are listed below and summarized in Fig. 9.10.

New synthesis methods:

- New mechanisms of polymerization, e.g., catalytic, enzymatic and free radical polymerization in dispersed media (emulsions, miniemulsions, etc) and under supercritical conditions
- Environmentally friendly methods using water as a solvent

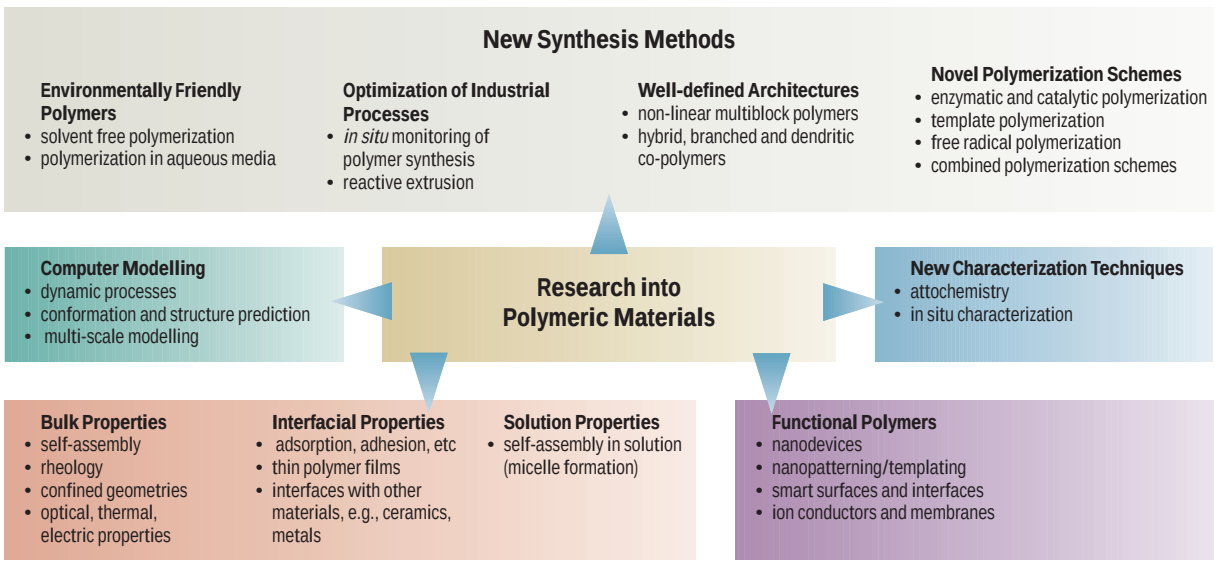

Fig. 9.10. Future research directions for polymeric materials.

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- Nanopatterning via block copolymer self-assembly
- Combining of polymerization methods or transforming of one active centre to another
- Selective solubilization of low molecular weight compounds
- High purity synthesis

Novel architectures and materials combinations:

- Composite materials for greater strength and functionality
- Behavior at polymer interfaces
- Nanostructured materials based on polymers

Functional polymers:

- Polymers for optics and electronics, e.g. light emitting diodes, displays, sensors, batteries
- Membranes for fuel cells and batteries
- Polymers for biomedical applications (see b) below)
- High performance polymers (polyimides, fluoropolymers, etc.)
- Organic-inorganic hybrid structures
- Smart materials for sensing and responding to environmental changes

Structure-property relationships

- Computer modelling from atomic to macro-scales
- Structural organization and design at the atomic/nano-level
- Transport phenomena in ion-conducting and gas filtration membranes
- High speed analytical techniques

(b) Bio- and biomimetic materials

Biomaterials is a rapidly growing field of materials research that has important implications for the quality of life of Europe's ageing populations. The main research priorities are:

- Understanding of the fundamental mechanisms of biomaterial-cell interactions and identificaiton of the quantifiable relationships between a material's surface characteristics and cell behaviour.
- Development of smart biomaterials that are able to sense tissue responses and release biological signals accordingly.
- Optimization of bone-bonding systems that can reliably and practically achieve stable fixation of prostheses to bone.
- Optimization of the architecture and microstructure of synthetic scaffolds to act as vehicles for three dimensional tissue regeneration.
- Development of systems that facilitate localized delivery of genes to diseased tissue.

Closely related to biomaterials are the biomimetics; these materials are synthesized by copying mechanisms and processes observed in Nature to provide optimal structures and properties. Biomimetics are used not only for medical purposes, but as structural, smart and functional materials also. Future research directions for both these fields are summarized in Fig. 9.11.

Europe is currently falling behind other regions in biomaterials research despite having the expertise and know-how. The strength of U.S. industry and size of its market is drawing many companies and researchers overseas. To remedy this situation, it is recommended that

- a database of implants, etc, be created to follow patient recovery over the long term.
- biomaterials be recognized as a legitimate field of research, e.g., by providing professorships, establishing university schools/departments.

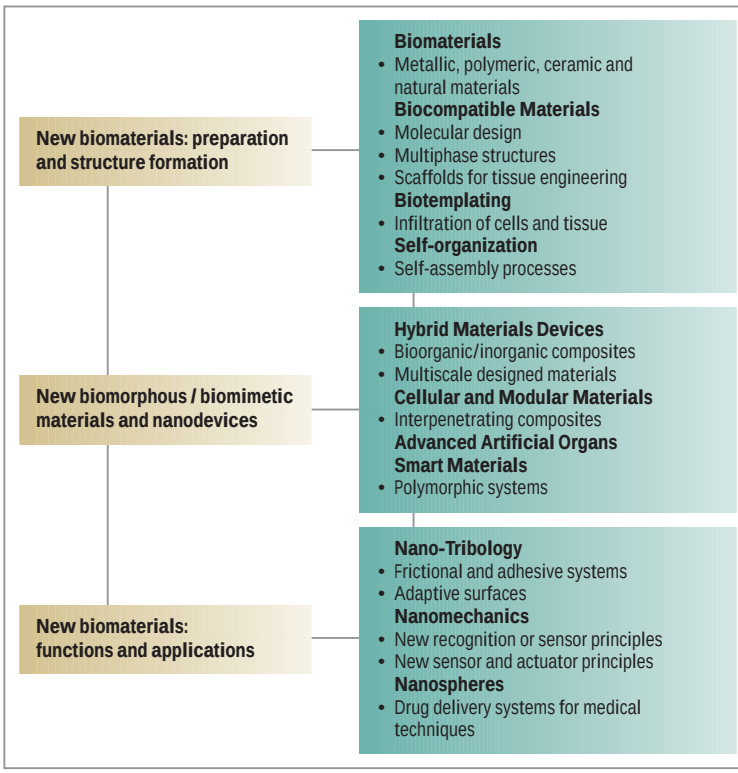

Fig. 9.11. Future research directions for bio- and biomimetic materials over the next decade.

- the EC convene multidisciplinary teams of experts to coordinate research efforts within the EU, and provide them with a boost in funding to establish biomaterials research centres specialising in different areas such as cardiovascular surgery, orthopaedics, ophthalmology.

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- protocols for discussing various ethical issues surrounding the development and use of biomaterials be established-regulatory bodies are needed to oversee research, particularly when patient trials are involved.

9.2.3. Nanomaterials

Almost all future materials science will be based on nanotechnological concepts. Materials will be able to be assembled layer-by-layer or even atom-by-atom to generate new atomic arrangements with completely new properties. Nanomaterials are designed (and are used) today in a variety of forms, such as nanopowders, colloids, thin films and coatings, multilayers and laterally structured systems (from nanostripes and nanodots in semiconductor research to nanopore filters made from polymers). We are already today able to connect semiconducting materials with magnetic, superconducting, organic and even biological materials with nanometre control. Nanoscale materials science is governed by three main phenomena: **confinement, proximity and organization**. The interplay of these three phenomena creates rich new areas for uncovering novel materials behaviour.

Nanotechnology promises to revolutionize the way we live and work, from manufacturing and medicine to computing and communications. Many new and clever combinations of materials, molecules, atoms and ions will emerge over the next few decades that display unusual and unexpected behaviour, thus allowing the development of tomorrow's devices and applications.

The confinement of materials to length scales below those producing ordinary macroscopic behaviour results in new spin and charge ground states, new electric and magnetic polarization textures, and new dynamics for polarization reversal and charge transport. Exchange of spin, charge, strain, electromagnetic fields, or matter across interfaces leads to novel proximity effects that profoundly affect the properties of neighbouring materials. These confinement and proximity effects can be precisely controlled through nanoscale organization, where the properties of hybrid materials are tuned by adjusting the feature sizes of the constituent materials. Fig. 9.12 summarizes key areas of research and applications in this field.

Future challenges in the science of nanomaterials:

- Nanoparticles, quantum structures, self-assembly materials and nanobiomimetrics demand priority attention in the near future.
- Do we know all possible mechanisms which lead to self-organized structures?
- Is it possible to stabilize at room temperature (STM-manipulated) structures consisting only of a few atoms?
- Possibilities of designing nanostructures using organic components (organic FETs, organic light-emitting devices, etc.) and nano-sized magnetic domains that allow high density data storage, exhibit tailored hysteresis

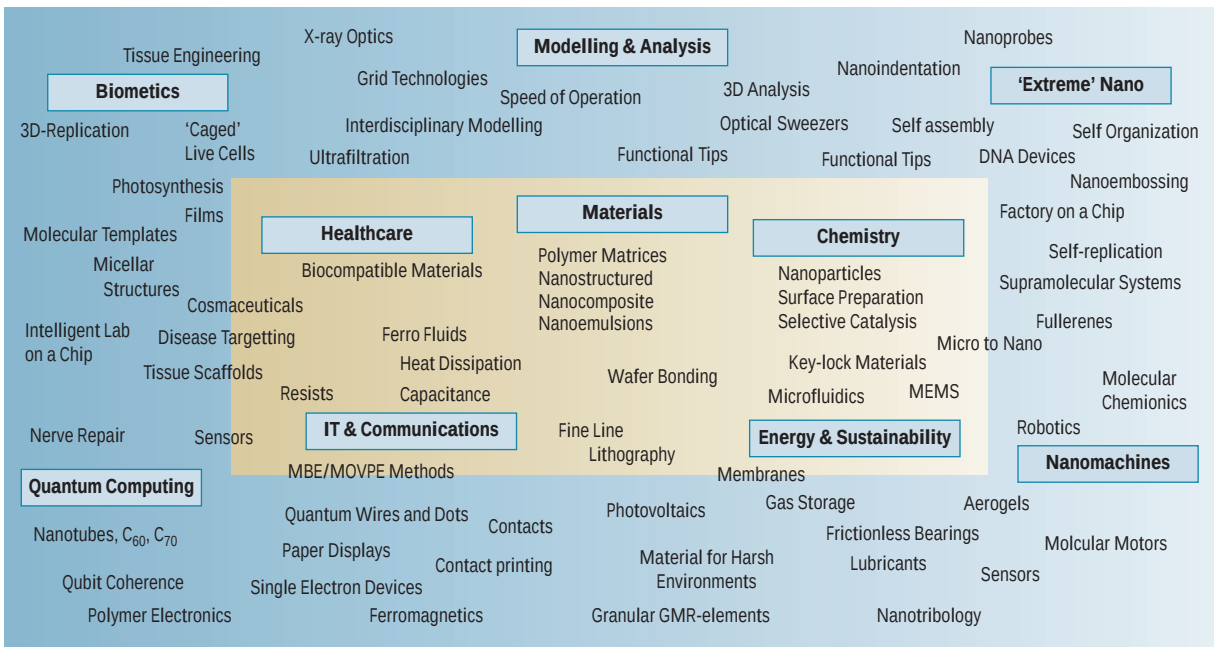

Fig. 9.12. A roadmap for nanomaterials research and applications in Europe.

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loops and can be switched at the highest speeds, need to be explored further.

- Further progress in spintronics depends on basic experimental and theoretical studies of ferromagnetic-semiconducting interfaces and nanostructures which preserve the electronic polarization.
- It is also important to realise that current technologies, particularly those based on semiconductor materials, are reaching their physical limits. Strong and coordinated basic research programmes are necessary now to come up with new ideas for overcoming these barriers.
- Nanotechnology is an essential part of any such strategy. For example, nanomaterials may open the door to new devices in the fields of quantum computing, quantum electronics, photonics and magnetics.
- Formation of quantum dots and wires of uniform size and distribution will be a demanding research field, as will be the fabrication of materials architectures and functioning circuits from these components to form useful devices.

Nanomaterials is by its very nature a multidisciplinary field bringing together experimentalists, theorists and engineers, physicists, chemists and biologists. The challenges of this are accordingly big. Communication between the various disciplines can be significantly improved via coordinated research programmes, particularly by establishing a nanomaterials network or centre of excellence. Europe must meet the challenge of creating the right balance of research and training infrastructure that can be accessed by scientists from all member states if it is to remain a technologically competitive into the future.

For Europe to become competitive in the field of nanotechnology it is imperative that:

- funding for basic nanomaterials research be increased to a level comparable to that in the U.S. and Japan, and nanotechnology and interdisciplinary research be given high priority in European materials programmes.
- interdisciplinary research centres dedicated to investigating nanomaterials and the applications listed in Fig. 9.12 are established.
- industry and academia work together to develop newer, more innovative synthesis and characterization techniques.
- research into self-assembly and biomimetic materials be increased.
- computer modelling be used to predict the properties and phenomena of nano-size particles and nano-designed materials.

9.2.4. Electronic, Optical and Magnetic Materials

Basic science in the fields of electronic, magnetic and optical materials involves understanding and controlling electrons and electronic correlations in materials and tailored materials structures. Over the last two decades this field has uncovered many fascinating new phenomena, e.g., the quantum Hall effect (QHE), giant magnetoresistance (GMR), high-temperature superconductivity, and the fractional quantum Hall effect (FQHE). Equally breath-taking is the speed with which most of these fundamental discoveries have entered today's technology, e.g., a new high-precision standard for defining the SI unit of resistance, the ohm (using QHE), new reading heads in hard disks (based on GMR), or new superconducting devices (from YBCO materials).

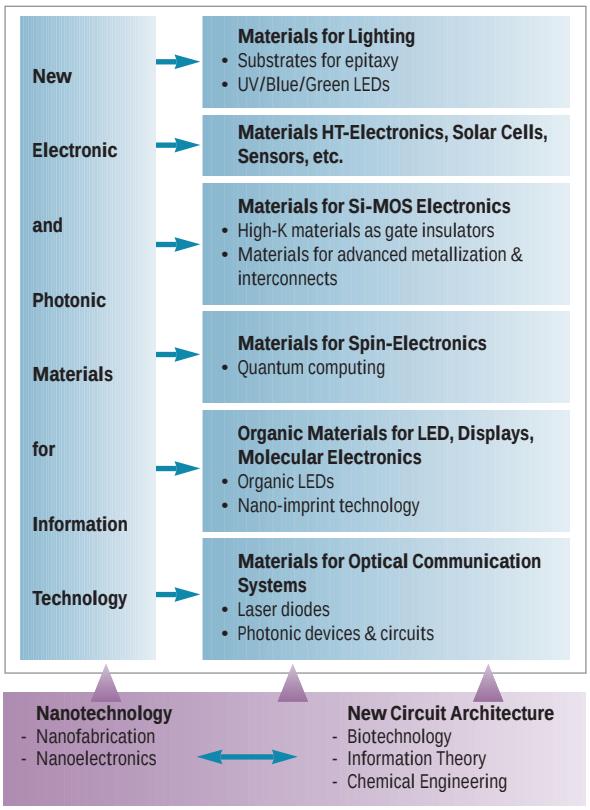

Fig. 9.13. Research and development of new materials for the Information Technology Summary of potential research areas with inputs from Nanotechnology and integration of novel architecture design concepts.

Electronic materials encompass a broad range of substances from semiconductors such as doped silicon, germanium and GaAs, to electronic and ionic conductors made of metals, polymers, and ceramics. Promising areas of research include organic semiconductors, nanostructured materials, quantum dots and wires, II-VI and III-V semiconductors, and self-assembling systems.

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Many breakthroughs have occurred in the use of **materials for optical applications**, especially lasers and communication devices. Novel organic materials, polymers and ceramics with tailored optical properties have all been developed. Optical materials research is one of the most innovative and rapidly developing fields of materials science and is continually resulting in new commercial products and discoveries.

A renaissance in basic research of **magnetic materials** is taking place as a result of breakthroughs in colossal magnetoresistance, magnetic multilayers, magnetic properties of thin films, magnetic coupling between layers, giant magnetoresistance and nanoparticle synthesis. This flourishing field of materials science is characterized by close collaboration between experimental and theoretical

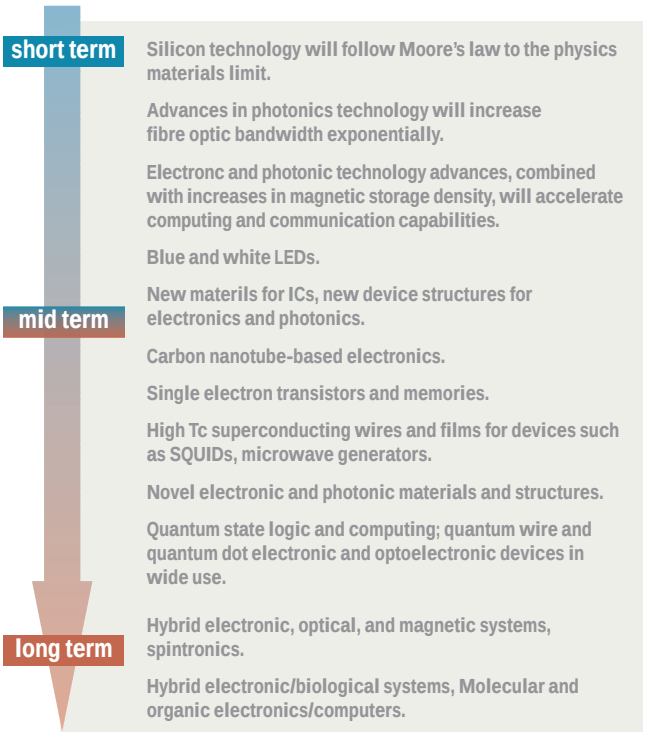

Fig. 9.14. Future progress in electronic, optical and magnetic materials in Europe

research groups. Breakthroughs are expected in the development of magnetic nanowires, perpendicular recording, magnetic non-volatile recording materials, magneto-optic layers, spin valves and molecular magnets. Most of these research activities are intimately related with nanotechnological and interdisciplinary concepts (Fig. 9.14).

Recent discoveries of **superconductivity** in MgB_2, polymers and high-pressure iron show that many surprises still await researchers in this area. The ceramic high temperature superconductors will find their first commercial application in the next few years, but the search for new higher temperature superconductors should also continue. In particular, further work needs to be done on

- optimizing microstructures and improving critical current densities,
- searching for new superconductors with small anisotropy and high critical temperature,
- developing and improving thin film deposition techniques,
- the detailed analysis of the materials at the micro- and nanometre scale,
- promoting exchange of scientific knowledge through creation of European networks.

A possible road map for European research in these areas is given in Fig. 9.14. In order to be able to follow this, several focused European actions are necessary:

- Establishment of interdisciplinary research centres for semiconductor technology that can compete with large research institutes in Asia and the U.S.
- Increase funding for research projects examining the fundamentals and application of single electron devices.
- Initiatives in electro-optic technology to develop next-generation computers and communications, particularly laser devices and photonics.
- Long-term projects to develop spintronics, quantum computing and other future technologies.
- Formation of Centres of Excellence in superconductivity to hasten the introduction of high temperature superconductor devices for use in industry, medicine and transport.
- Greater industry-academia collaboration on ways of improving/optimizing electronic storage media and other devices based on recent breakthroughs in magnetic materials.

9.2.5. Materials Applications and Related Topics

Advanced materials are used in a diverse range of new and established technologies that underpin our current standard of living, and will make future technologies possible. While there is not enough room to discuss all of these here, a few examples are given of promising and topical, but also less well-known, areas of research to illustrate the diversity of needs for modern materials technology.

(a) Materials for catalysis

In order to maintain and strengthen the world-wide leading position of European catalysis science and industry, a next generation technology platform for advanced catalysis research should be created, bearing in mind the need for full integration of homogeneous, heterogeneous and

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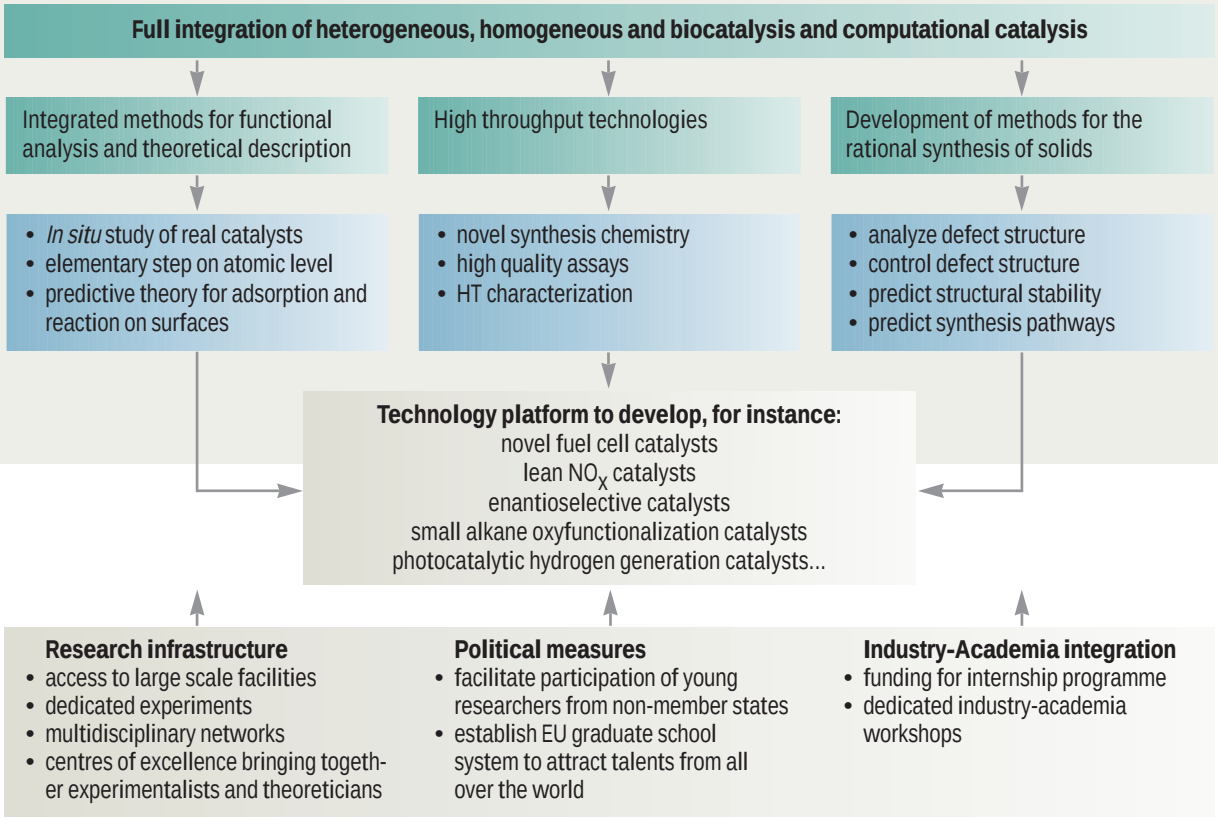

Fig. 9.15. Future research directions for catalytic materials.

biocatalysis, and including computational methods as an essential part. This technology platform should provide the enabling technology package for accelerated materials development in catalysis on the basis of an improved understanding of the controlling parameters and the processes which control these parameters on a fundamental level. The application of these enabling technologies will lead to new generations of catalysts for processes decisive for a sustainable development (Fig. 9.15). The interplay of the different factors and the role of EU actions is summarized in the following diagram.

Research topics at the forefront of catalytic science include:
- Selective oxidation
- Environmental catalysis
- Asymmetric catalysis
- Combinatorial catalysis

Recommendations for catalysis research in Europe include:
- basic research into novel materials and catalytic mechanisms at the atomic level.
- environmental legislation encouraging greater use of catalysts for pollution reduction and efficient processing.
- greater industry-academic collaboration on promising catalytic systems.
- establishment of a interdisciplinary European Catalysis Institute or Network of Excellence (see Annex 1 in Chapter 8).

(b) Materials for fusion reactors

Fusion technology promises to provide a limitless supply of clean and cheap electricity. Its success strongly depends on the availability of high quality structural materials that can withstand extreme environments. Over the last thirty years, however, fusion research has conducted mostly by the engineering community, and materials improvement has been limited. Fundamental research will be vital for overcoming current materials limitations. The development of fusion materials would be expediated by greater interaction between fusion scientists and materials scientists.

(c) Materials for transportation

The transportation industry places extraordinary demands on the properties, performance and cost of materials because of considerations of safety, reliability, economy and design. To attain commercial success, materials engineering requires the simultaneous optimization of all these factors during the conversion of raw materials into products. The core purpose of this rigorous process of simultaneous engineering is to achieve an optimal balance between cost and product per-

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formance. It is therefore recommended that Europe establish strategies for simultaneous development and engineering of materials including, among other things:

- rapid analysis techniques for complex systems
- materials with improved reliability or self-repair capabilities
- light-weight and energy-efficient materials
- smart materials for responding to vehicle conditions and providing passenger comfort.

(d) Materials research in space

Space platforms offer the unique opportunity to probe materials, phenomena and processes in zero-gravity environments. This space-based materials research is potentially important for container-less studies and processes, for basic studies of diffusive crystal growth, for the growth of semiconductors with low defect densities or for the solidification of metals and glasses which may result in improved casting technologies. The apparent drawback of such experiments are the very high costs and risks involved. It is thus recommended

- to further develop a European space-based materials science programme in a thoughtful manner which includes a careful analysis of the objectives and success probability of the individual materials science projects. For microgravity studies which can be carried out within a couple of seconds it is also advisable to consider ballistic rockets and fall towers as alternatives.

9.3. Materials Interdisciplinarity

Materials science is by nature an interdisciplinary field, traditionally spanning engineering, chemistry and physics. The future of materials science will be in the further integration of other disciplines such as biology, medicine and computing. Knowledge from these fields will hasten the development of materials science, resulting in new technologies, innovations and applications, e.g., organic computers. At the same time, the breadth of materials science and the phenomena it encompasses can only be understood if researchers in different disciplines collaborate to generate new insights and help solve problems. To foster interdisciplinary research, institutions should adopt a flexible structure with close contact and good communications between departments and disciplines.

Some of the most promising areas of interdisciplinary research in materials science are:

- Bio-, biomimetic and self-assembly materials
- Nanomaterials
- Computer modelling (especially multi-scale modelling)
- Smart materials
- Surface and interface science

As an example, Fig. 9.15 shows how surface and interface science acts as an interdisciplinary platform. Our ability to control the structure of interfaces on the atomic level has made it possible to create many new and fascinating interfacial structures. Solid-solid interfaces in magnetic multilayer materials result in unusual magnetic properties (e.g., the giant magnetoresistance effect). A current topic of great scientific interest and high application potential is the study of interfaces between ferromagnets and semiconductors, with the objective of controlling the injection of polarized electrons into semiconducting devices. Interfaces between metals or semiconductors on one side and organic materials on the other opens up completely new fields in functional coatings and organic semiconducting devices. The controlled oxidation of surfaces may produce new nanometre-sized dielectric and tunneling barriers required for future developments in the semiconductor industry.

None of these projects in surface and interface science would be possible without close collaboration between physicists, materials scientists, chemists and (more recently) biologists. It can safely be predicted that future research will reveal novel structures, phenomena and properties which do not exist naturally and which open up the possibility of completely new functionalities.

The five research areas listed above are by no means distinct, and will also bear upon one another in an interdisciplinary manner; e.g., biomaterials designed at the nanolevel (i.e. bionanotechnology) could be used in the next generation of smart devices. The materials developed through interdisciplinary collaboration promise to revolutionize industrial, medical and information technologies, and thus bring enormous benefits in terms of improved standards of living. Two ways of fostering interdisciplinary

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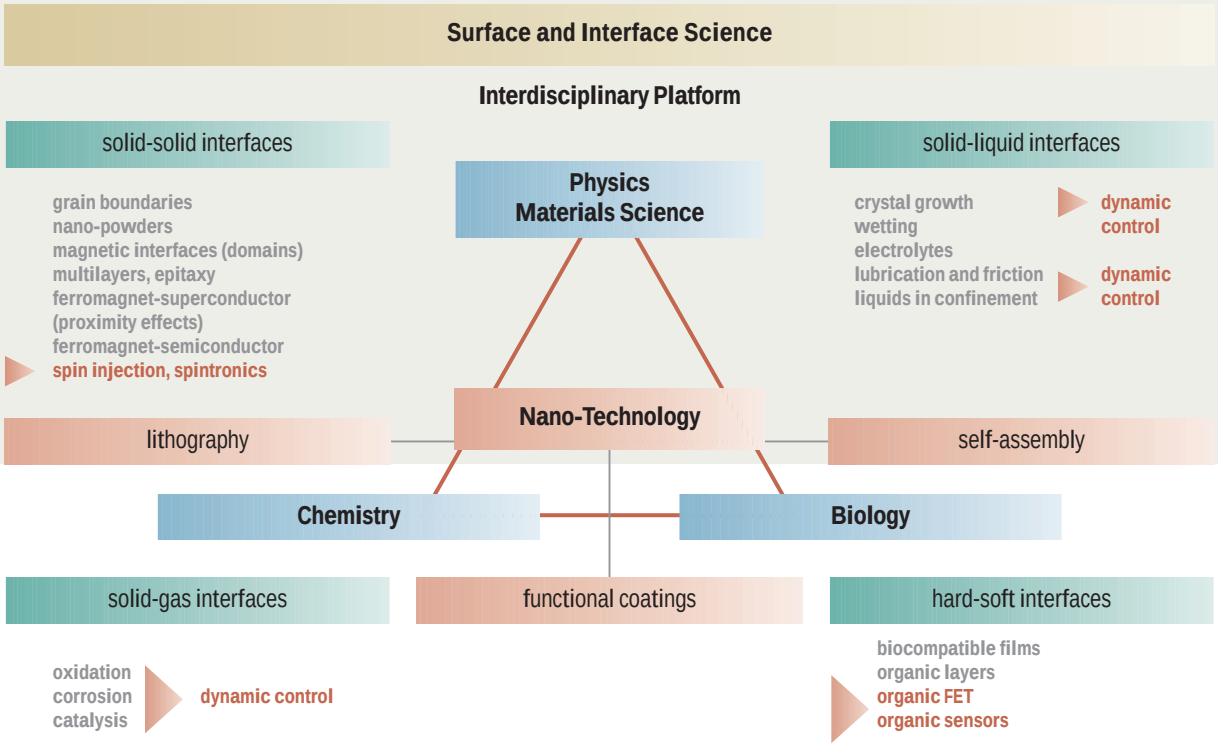

Fig. 9.15. The interdisciplinary approach to surface and interface science.

research are: i) establishing research institutes or labs in which researchers from two or more university departments or disciplines tackle related problems, and ii) linking researchers and institutes from different disciplines via networks to enhance communication and guide research in new interdisciplinary fields. Training programmes should also be highly multidisciplinary in outlook so that researchers have a flexible range of skills and can make new connections between different fields.

It is therefore imperative that:

- interdisciplinary research programmes in materials science are initiated on a European level,
- interdisciplinary European workshops, training programmes and summer schools are organized,
- interdisciplinary European research networks are set up,
- funding agencies for different branches of science coordinate their activities to make it easier for interdisciplinary projects to be established.

9.4. New Research Strategies and Infrastructures in Europe

9.4.1. Social Acceptance of Science

Steps need to be taken to reverse the trend of decreasing numbers of students in materials science courses at university, and the alienation of many members of the public from science in general. These multi-faceted issues need to be tackled from as many different angles as possible:

- restore public confidence in science by using publicly-funded science for the public good;
- improve teacher training and school curricula to make science exciting and attractive to pupils in primary and secondary education;
- engage the public on scientific issues of social relevance through TV programmes, live debates, science fairs and other events;

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- improve career structures and salaries for research scientists (see below) to attract more students;
- broaden science courses to include issues of social relevance, ethics and better communication skills.

9.4.2. Political Support for Science

Many areas of materials science require substantial investment and support to perform cutting-edge experiments with world-class equipment and facilities.

- European governments need to increase funding for basic science to levels similar to those in Japan and the U.S. if their economies are to remain strong in the 21st Century.
- Breakthroughs in materials science are essential for biotechnology, IT and other technologies that will determine our quality of life in the future. Materials science should therefore receive similar funding levels to these boom areas.
- Academic scientists need to be better represented at national and European levels, and should have a larger say in the science policy of the EC and Member States.

9.4.3. Materials Science and Education in Europe

(a) Basic science education

The excitement and rewards of studying basic science need to be conveyed to youngsters as early as possible to ensure that tomorrow's Europeans value science and more of them take it up as a career. Initiatives to do this should include:

- science training and refresher courses for primary and secondary school teachers,
- visits to labs and large-scale facilities performing cutting-edge research,
- scientists visiting schools to talk to children about the adventure science, careers in science and scientific issues.

(b) Role of universities

Although collaboration with industry is important, the primary function of universities should be to educate students and perform innovative and horizon-broadening research. With renewed funding from their respective governments, materials science departments throughout Europe would be able to refurbish buildings and update equipment so as to attract more students and increase research output. Universities also need to be flexible enough to establish new interdisciplinary, interdepartmental centres for working on the scientific fields of tomorrow, such as biomaterials, smart materials and nanoscience.

(c) Human capital and research careers

Europe has enormous potential for generating innovative ideas and new technologies because of its cultural diversity and long tradition of doing top-class science. In order to realise this potential, increased mobility of researchers, particularly within the EU, is essential. Information about research opportunities in other countries should be distributed more widely, the number of international researcher fellowships increased, and restrictive immigration laws or university employment policies relaxed. Career structures and salaries for research scientists should also be improved, e.g., by encouraging universities to provide more tenured positions rather than taking on postdocs. To meet industry's demands for more materials scientists and engineers, and to reflect changes and progress within society, more women and minority group students should be encouraged to take up materials science as a career.

9.4.4. Training, Mobility and Public Relations

In order to attract talented young people back to basic science and research, fundamental changes in researcher training and academic career structures are needed. European universities and research laboratories need to provide:

- more competitive salaries;
- more attractive career options for young people, including job security;
- more women students and lecturers/professors.

Greater mobility of researchers, particularly within the EC, should be encouraged to foster professional development and cross-fertilization of ideas. This would be greatly assisted by the creation of a European-wide qualification for materials scientists (EurMat) similar to that already existing for physicists (EurPhys).

As well as learning technical skills, European researchers should also receive foreign language training and communication skills. The latter is especially important if scientists are to communicate effectively with and convey their thoughts and motivations to an increasingly skeptical public. For materials science and related technologies to prosper in Europe, better promotion of this field as a discipline/career and improved public relations are vital.

9.4.5. New Strategies for Basic Research in Europe

(a) Overall strategies

Europe should aim to be number one in as many new materials technologies as possible. It is vital that European governments and the EC coordinate research efforts via

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European-wide materials science programmes and networks

- The EC should recognize the central role of materials science for technological development in its planning, funding and coordinating activities.
- The EC should set up a European Materials Council to work together with national materials societies, institutes and research councils to ensure that Europe develops first-class facilities, and to respond to the more specific needs identified in this White Book.
- Research strategies for materials science should include both small-scale and large-scale projects to take into account the needs of different Member States and research fields:

(b) European research networks

Creating research networks will allow a "critical mass" of researchers to be brought to bear upon complex, large-scale problems, particularly interdisciplinary areas such as nano- and biomaterials. These networks could be formalized as virtual research centres or Networks of Excellence, funded by the EC, and consisting of research groups and laboratories from throughout the EU. The growth of the Internet should also be utilized to provide high speed communications. This would allow faster flow of information, better sharing of resources, and efficient allocation of expertise for teaching and guiding and evaluating projects.

(c) Research facilities

Europe already has excellent experience in successfully managing and operating large-scale facilities. The number of large-scale research facilities accessible to materials scientists should be increased in the medium to long term in order to attract the world's best scientists and raise the standard of European research even higher. Recommendations concerning new EC-managed facilities are:

- Centres of Competence and Centres of Excellence in Materials Science and Technology should be established around Europe to house the latest apparatus and develop new analytical techniques.
- Small- and medium scale laboratories should upgraded with modern in house instrumentation
- High Resolution Electron microscopy and High Resolution Laser and NMR spectroscopy centres need to be defined or created
- Training programmes should be offered to researchers, technicians and engineers to ensure resources are maintained and used most efficiently.
- R&D into fourth generation (LINAC-driven) synchrotron sources and pulsed neutron sources should further be pursued with the aim of constructing and running a large-scale facility over the long term.

(d) International collaboration

International collaboration is a vital part of modern science:

- Materials scientists should be encouraged to spend time overseas in other cultures and research environments in order to bring their newfound knowledge back to Europe.
- Nationals from regions outside of Europe should be encouraged to work in Europe through generous fellowships and research positions.
- International conferences should be held regularly and attended by researchers at all stages of their careersas they sew the seeds for new innovative ideas and fruitful research collaborations.

9.5. Closing Remarks

Major breakthroughs in materials science are expected over the next decade, revolutionizing the way we manage and interact with our environment. Europe must utilize its resources efficiently and maintain a critical mass of expertise to continue at the cutting-edge of research. Equally important is the promotion of materials science education and careers to the younger generation.

This White Book is intended to show the fundamental importance of basic research in materials science to modern technology, and predict the directions it will take us in the future. As the driver behind many of today's high-tech industries, materials science deserves the full support of research councils, governments and the general public.

It is hoped that the recommendations in this book will be implemented so that European materials science and industry prosper well into the 21st Century. It is the responsibility of educators, scientists, politicians, and other professionals to ensure that Europeans grab hold of the enormous opportunities that these developments in materials science present.

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Max-Planck-Institut für Metallforschung Stuttgart, Germany

EU-Workshop
on Strategies for Future Areas of Basic Materials Science

H. Dosch, E. Mittemeijer, M. Rühle, M.H. Van de Voorde

June 13 - 15, 2000
Schlosshotel Monrepos | Domäne Monrepos 22 | 71634 Ludwigsburg

Schedule of Workshop

	June 13	
12:00-13:00	*lunch*	
13:00-13:30	Welcome and introduction to the objective of this workshop	(Rühle)
13:30-16:00	Session on Materials	(Raabe, Eberl, Aldinger, Wegner)
16:00-16:30	*coffee break*	
16:30-18:30	Session on Materials	(Raabe, Eberl, Aldinger, Wegner)
19:00	*dinner*	
20:30-22:30	continue Materials, start Phenomena, or general discussion	
	June 14	
08:30-10:00	continue session on Phenomena	(Kirschner, Arzt, Mittemeijer, Parrinello)
10:00-10:30	*coffee break*	
10:30-12:30	continue session on Phenomena	(Kirschner, Arzt, Mittemeijer, Parrinello)
12:30	*lunch*	
14:00-16.00	Session on Characterization	(Dosch, Rühle)
16:00-16:30	*coffee break*	
16:30-18:30	Session on Characterization	(Dosch, Rühle)
19:00	*dinner*	
20:30-22:30	Session on Processing	(Jansen)
	June 15	
09:00-10:30	Workshop Summary and Discussion on general issues and on further action	
10:30-11:00	*coffee break*	
11:00-12:30	Workshop Summary and Discussion on general issues and on further action	
12:30	*lunch*	
13:30	End of workshop	

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Working Group	Topics	Discussion leader	Participants
Materials	Metals and Alloys, Composites	Raabe	De Hosson, Gottstein, Gösele, Vitek, van Houtte
	Semiconductors	Eberl	Forchel, Ploog, Madar
	Ceramics and Ferroelectrics	Aldinger	Baumard, Flükiger, Maier, Waser
	Soft and Bio-Materials, Interfaces	Wegner	Bonfield, Ciardelli, Hadjichristidis, Hadziioannou, Johannsmann, Schmidt, Vidal
Phenomena	Electronic Correlations	Kirschner	Buschow, Fulde
	Small-Scale Materials	Arzt	Borghs, Gao, Prinz, Spaepen
	Solid-Gas, -Liquid, -Solid Reactions	Mittemeijer	Agren, Howe, Schlögl
	Modelling and Theoretical Physics	Parrinello	Dietrich, Kremer, Neugebauer, Pettifor
Characterization	Diffraction and Spectroscopy	Dosch	Deville, Clausen, Findenegg, Kaindl, Keimer, Kunz,Louer, Miranda, Richter, Schneider
	Microscopy and Probe Techniques	Rühle	Bolt, Colliex, Smith, Urban, van Tendeloo
Processing	Materials Synthesis	Jansen	Barboux, Etourneau, Kniep, Rey, Schüth

Working groups should address the following issues: (a) state of the art 2000 +; expected trends 2000-2010 without focussed action; (b) expected needs 2002-2015: worldwide and EU (c) action to be taken in order to achieve (b); worldwide and EU needs could encompass: new initiatives, new materials, properties, new facilities, more manpower, interdisciplinary programmes, etc.

APPENDIX II

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Presentation of
EC White Book on Fundamental Aspects in Materials Research

H. Dosch, E. Mittemeijer, M. Rühle, M.H. Van de Voorde

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Agenda

	Thursday, March 15	
17.00		General Discussion
	Chair: Helmut Dosch (Stuttgart)	
ca. 19.30		Buffet Dinner
	Friday, March 16	
08.30	Eduard Arzt (Stuttgart)	Welcome
08.40	Manfred Rühle (Stuttgart)	Introduction and General Overview
	Presentation of the White Book	
	General Materials Classes	
09.10	Jean Etourneau (Bordeaux)	Inorganic Materials
09.30	Piet Lemstra (Eindhoven)	Soft Materials
09.50	Klaus Ploog (Berlin)	Functional Materials
10.10	Thomas Elsässer (Berlin):	New Research Tools
10.25	Huajian Gao (Stuttgart)	Materials Theory
10.40	*Coffee Break*	
	Specific Materials	
11.15	William Bonfield (Cambridge)	Bio-Medical Materials
11.25	Ferdi Schüth (Mülheim a.d.R.)	Catalysis Materials
11.35	Harald Bolt (München)	Fusion Materials
11.45	Helmut Kronmüller (Stuttgart)	Magnetic and Superconducting Materials
	Cross-Disciplinary Activities	
11.55	Eduard Arzt (Stuttgart)	Small Scale Phenomena
12.15	Wolfgang Pompe (Dresden)	Interdisciplinarity
12.30	Conclusions	
13.00	*Lunch*	

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