Edward DeMille Campbell

1863-1925

This annual lecture was inaugurated in 1926 in memory of the outstanding scientific contributions to the metallurgical profession by a distinguished educator who was blind for all but two years of his professional life. Despite this handicap, he contributed 77 papers to the scientific literature, the majority of which dealt with a correlation of the chemical constituents with the physical and mechanical properties of steels. This lecture recognizes demonstrated ability in materials science and engineering. Professor Campbell, Honorary Member of ASM International, was born in Detroit, Michigan in 1863, and was educated at the University of Michigan. After serving as a chemist in various iron companies, he became an Assistant Professor at the University of Michigan in 1890 where he lost his sight at the age of 28 in an explosion during a laboratory examination of steel. For 20 years before his death in 1925, he was Head Professor of Chemistry and Metallurgy and Director of the Chemical Laboratory at the University of Michigan.

COMPUTATIONAL MATERIALS SCIENEERING

G.B. Olson

Northwestern University & QuesTek Innovations LLC

Evanston, Illinois

2006 Edward DeMille Campbell Memorial Lecture

MS&T'06

Cincinnati, Ohio

October 17, 2006

NORTHWESTERN UNIVERSITY

QUESTEK INNOVATIONS LLC

MTL/SRG

A) Cybersteel 2020 (ONR D3D/Grand Challenge)
B) HT Carburizing Steels (DOE-OIT; GM, P&W)
C) Superalloys (DARPA-AIM; AF-MEANS, RMCI, MDT)
D) Bulk Metallic Glasses (DARPA-SAM)

GOVERNMENT

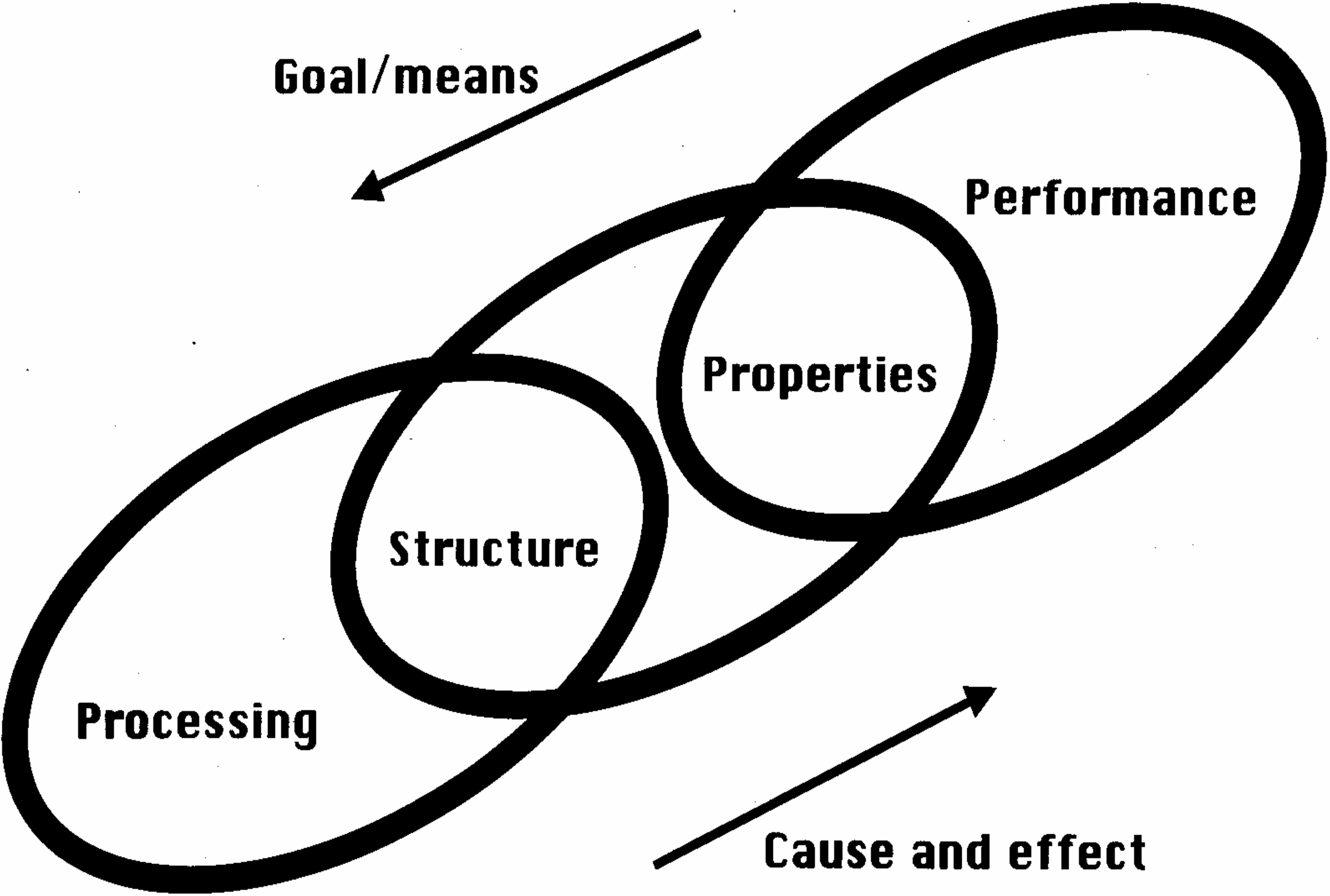
Organization	Members	Programs
NAWC/AD	Lee	A
NRL	Spanos	A
ARL/WMD	Montgomery	B
AFRL	Woodward, Miracle	C,D
LEHIGH	Harlow	C
WISCONSIN-MAD	Perepezko	C,D
IIT	Nash	D
VIRGINIA	Poon	D

UNIVERSITY

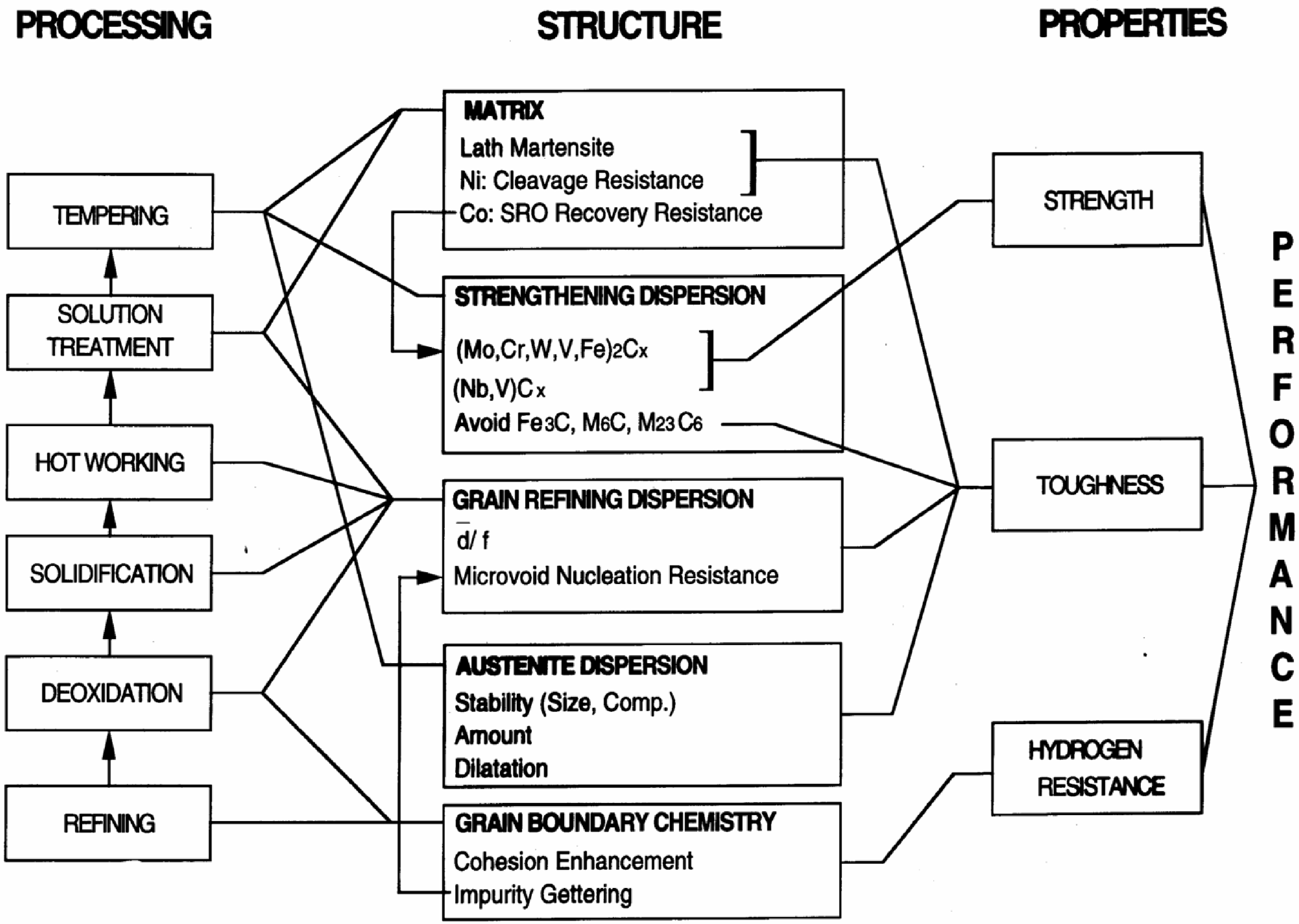
Organization	Members	Programs
NORTHWESTERN	Olson, Isheim, Brinson, Jerome, Espinosa, Liu, Fine, Moran, Freeman, Voorhees; High Resolution Microanalysis	A,B,C,D
GIT	McDowell	A
MICHIGAN	Pollock	A
CSM	Eberhart	A,C
OHIO STATE	Fraser, Mills	A,C
MIT	Parks	A,D
WPI/CHTE	Apelian	B
PURDUE-CALUMET	Abramowitz	B
KTH (Stockholm)	Agren	C

INDUSTRY

Organization	Members	Programs
QUESTEK	Kuehmann, Kern, Rathbun, Wang, Huang, Jung, Tang, Wright, Jou, Misra, Tufts	A,B,C,D
CATERPILLAR	Chen, Johnson	A,B
ALLVAC STEEL	Lippard	A,B
INLAND STEEL	Bhattacharya	A
GM	Mishra, Sachdev	B
FORD	Li	B
BOEING	Bowden	B,D
PRATT & WHITNEY	Fowler, Schirra, Watson	B,C,D
MEDTRONIC	Adler, Lesser	C
REFERENCE METALS	Carneiro	C
HOWMET	Wolter	D

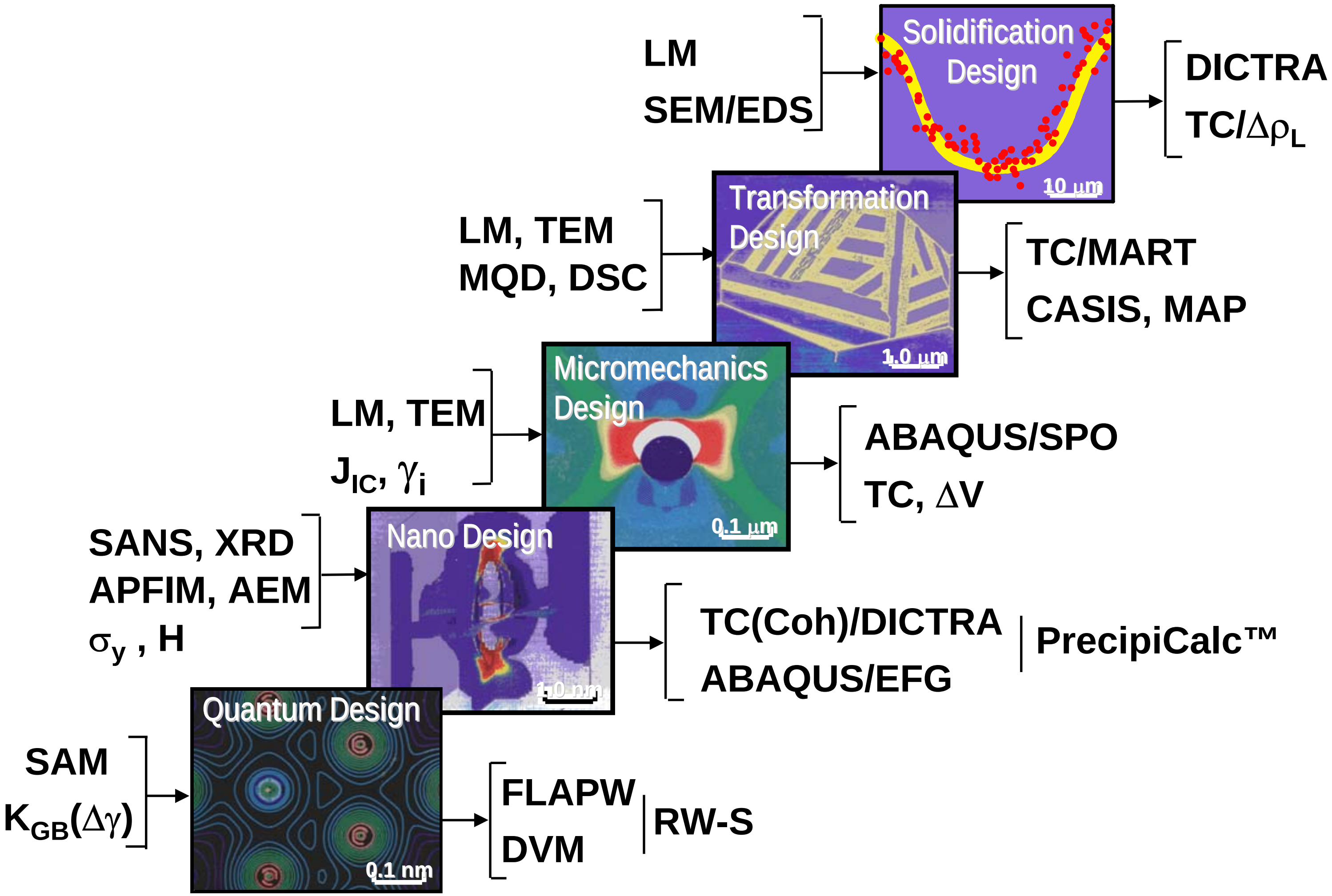


Goal/means
Performance
Properties
Structure
Processing
Cause and effect

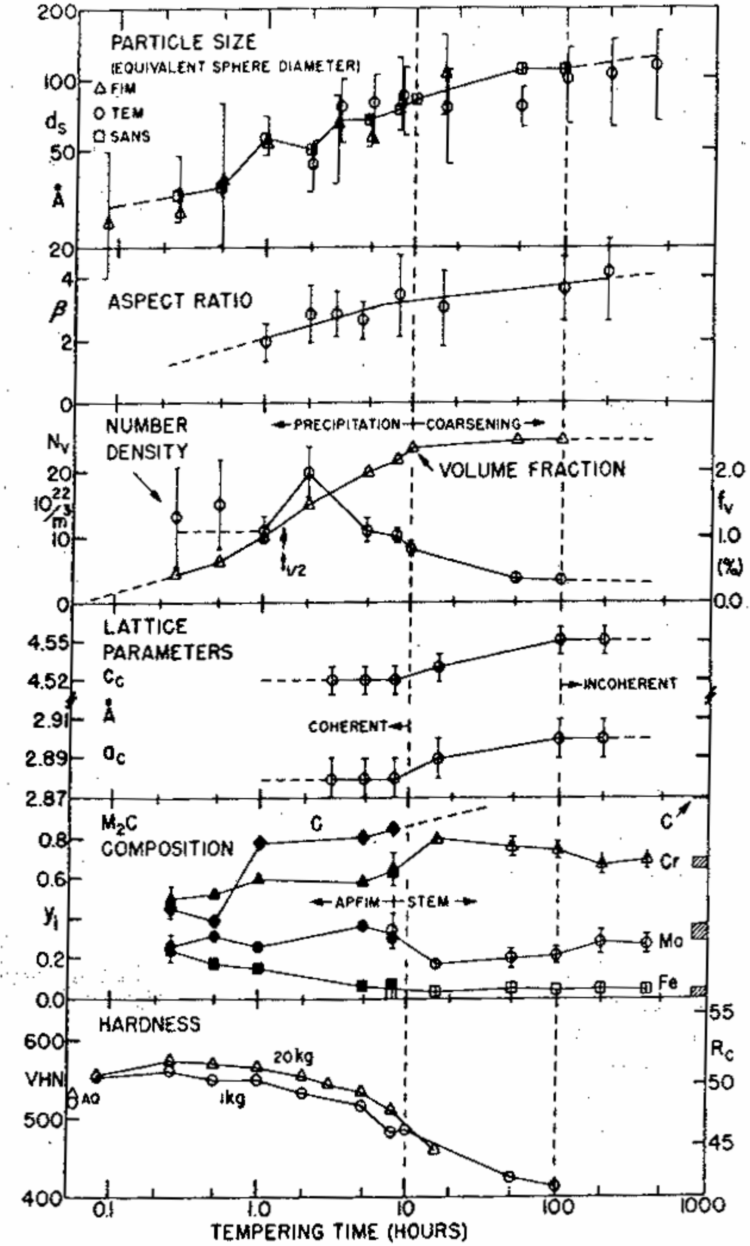


PROCESSING
STRUCTURE
PROPERTIES
TEMPERING
SOLUTION TREATMENT
HOT WORKING
SOLIDIFICATION
DEOXIDATION
REFINING
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
STRENGTHENING DISPERSION
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
GRAIN REFINING DISPERSION
d/ f
Microvoid Nucleation Resistance
AUSTENITE DISPERSION
Stability (Size, Comp.)
Amount
Dilatation
GRAIN BOUNDARY CHEMISTRY
Cohesion Enhancement
Impurity Gettering
STRENGTH
TOUGHNESS
HYDROGEN RESISTANCE
PERFORMANCE

Hierarchy of Design Models



M2C Precipitation

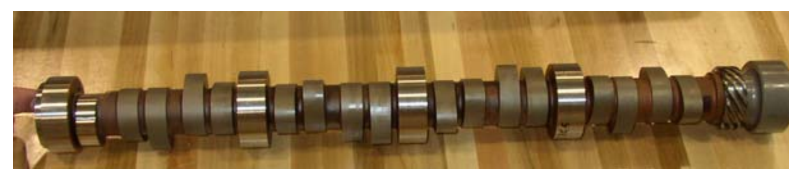


M2C carbide precipitation behavior in AF1410 steel vs. tempering time at 510C following 1 hour solution treatment at 830C

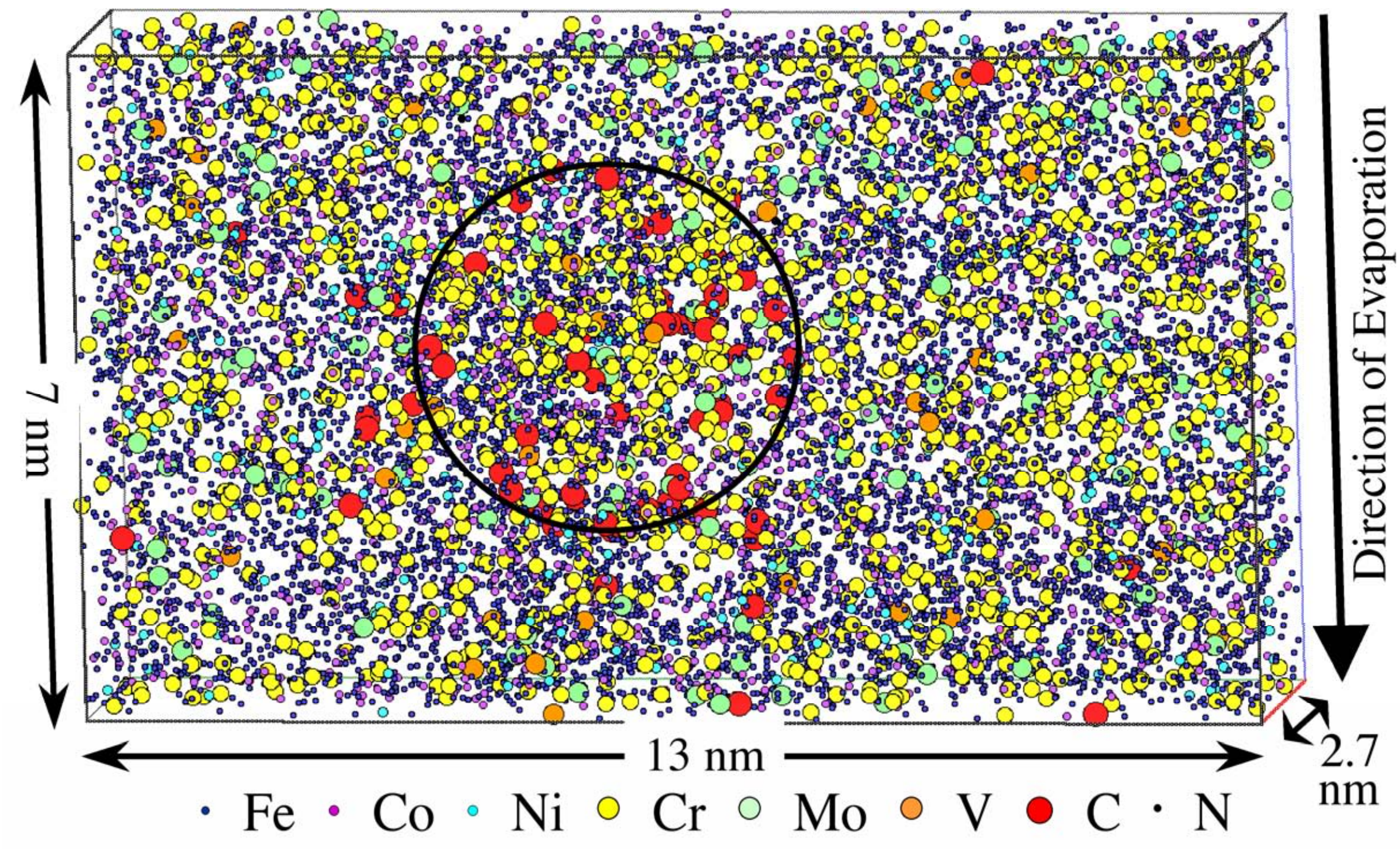
Current sales Ferrium® C61

Ring and Pinion

Camshafts

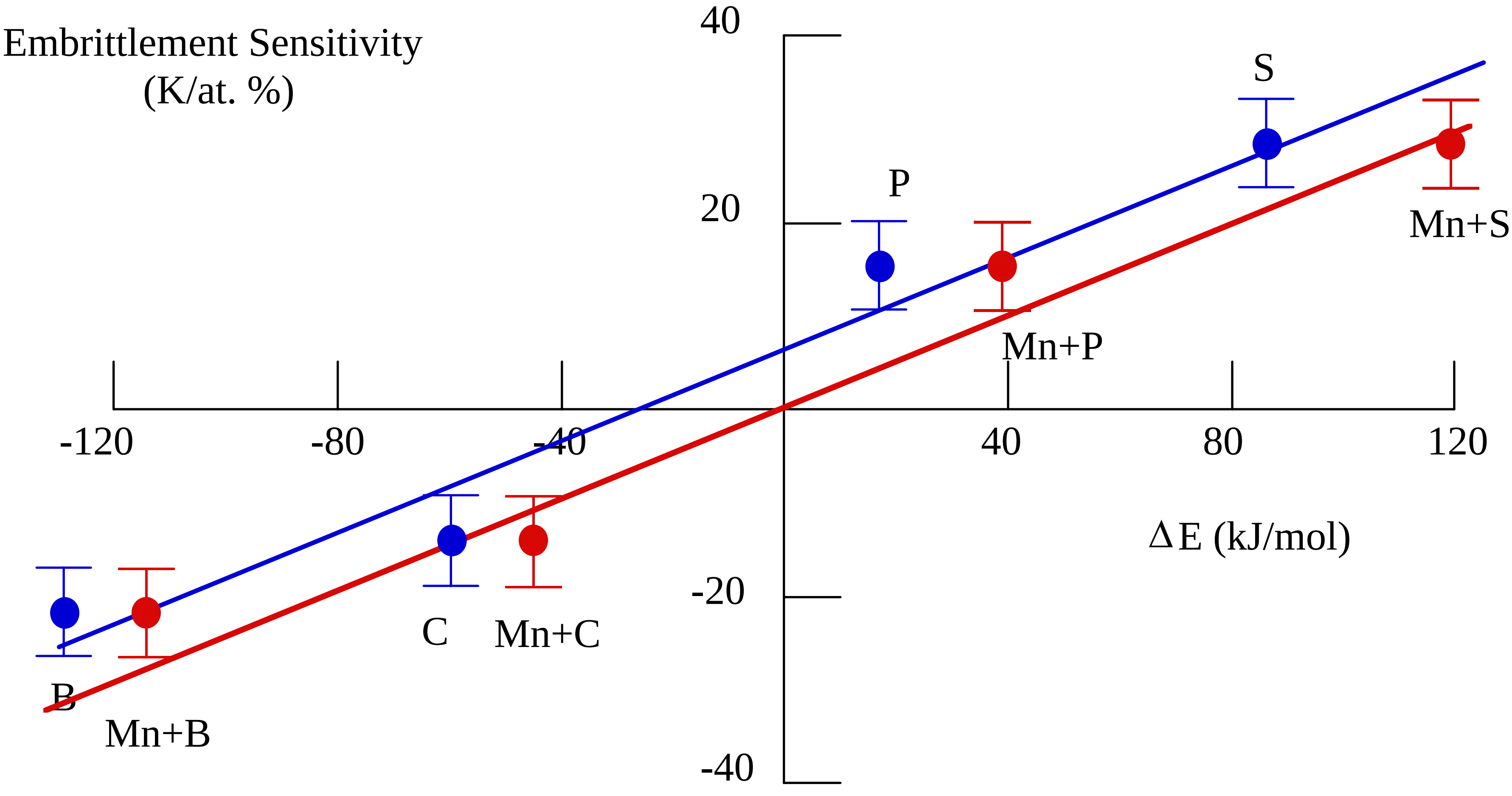


S53: Nanotechnology Now

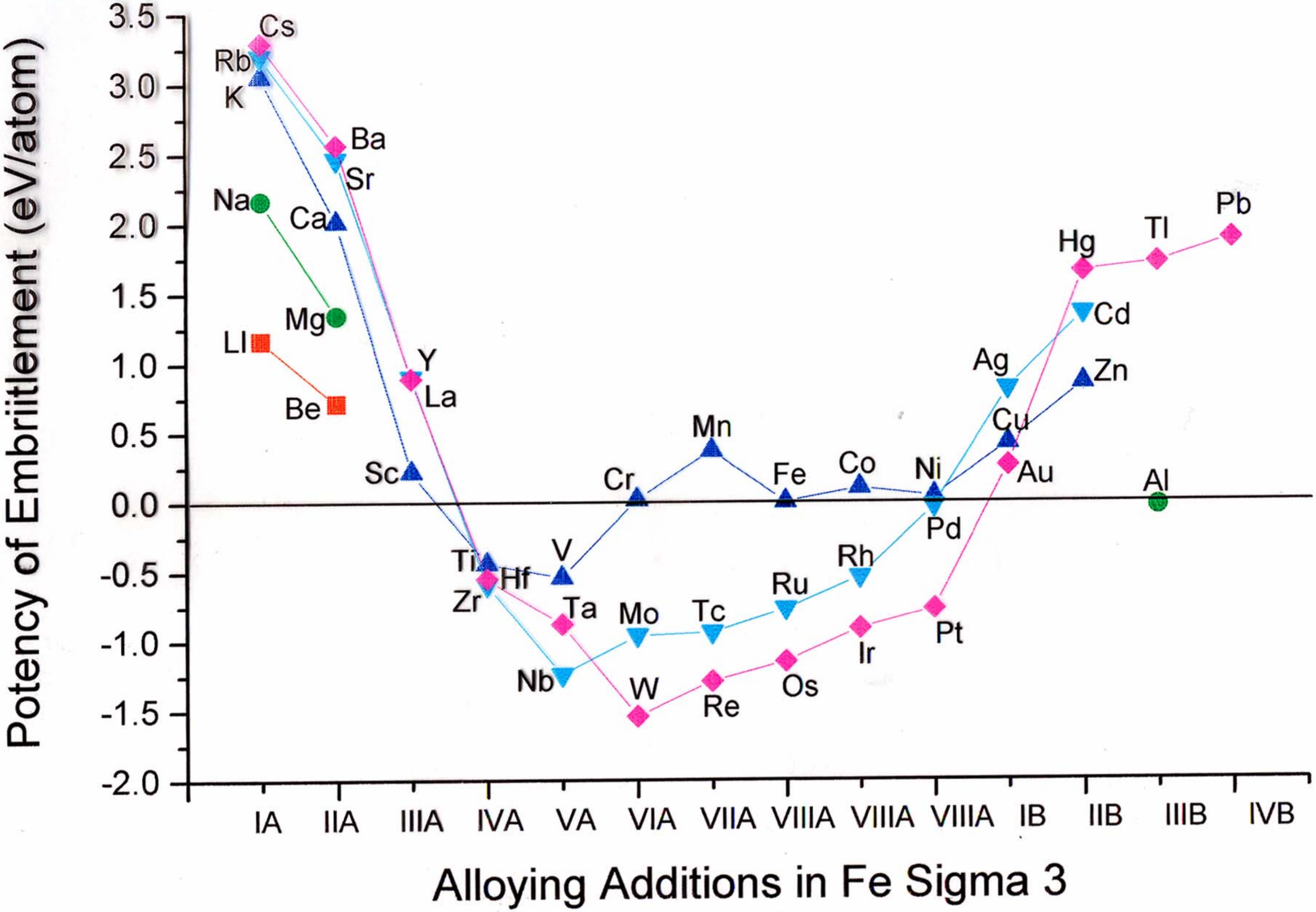



671

Grain Boundary Embrittlement

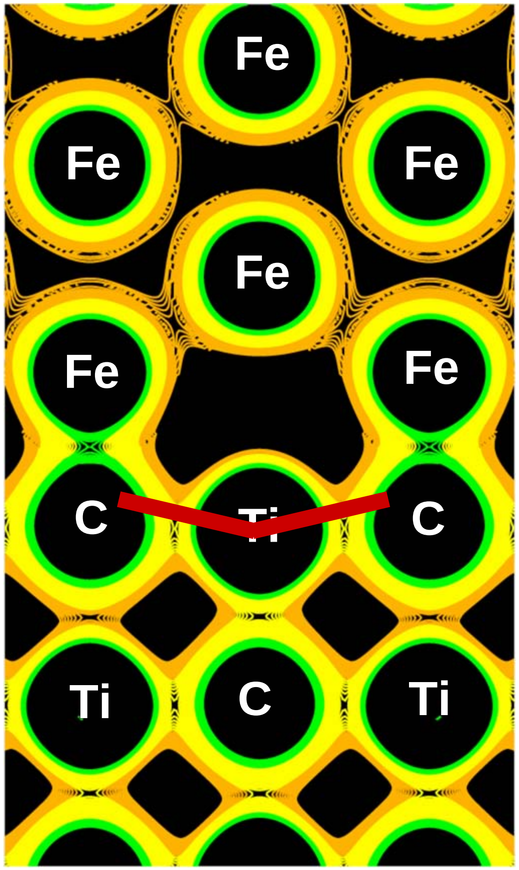


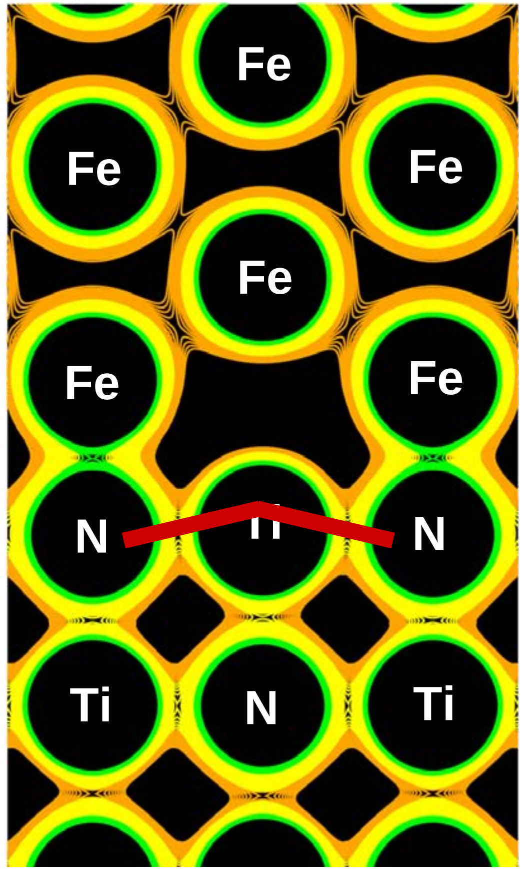
J.R. Rice and J.-S. Wang, Mater. Sci. Eng., 1988



Potency of Embriitlement (eV/atom)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Cs
Rb
K
Ba
Sr
Na
Ca
Mg
LI
Be
Y
La
Sc
Ti
Hf
Zr
V
Ta
Nb
Cr
Mo
W
Mn
Tc
Re
Fe
Ru
Os
Co
Rh
Ir
Ni
Pd
Pt
Ag
Cu
Au
Hg
Cd
Zn
Tl
Pb
Al
IA
IIA
IIIA
IVA
VA
VIA
VIIA
VIIIA
VIIIA
VIIIA
IB
IIB
IIIB
IVB
Alloying Additions in Fe Sigma 3

Charge Density : Fe/Ti[C,N]





- **Strong covalent feature**
- **Short bonding distance**

  Fe-C : 1.88 Å

  Fe-N : 1.90 Å

  (cf) Fe_3C : 1.94 Å

- ***Opposite buckling***

  Fe/TiC : 0.07 Å

  Fe/TiN : 0.07 Å

- **Same maximum charge density in the bond**

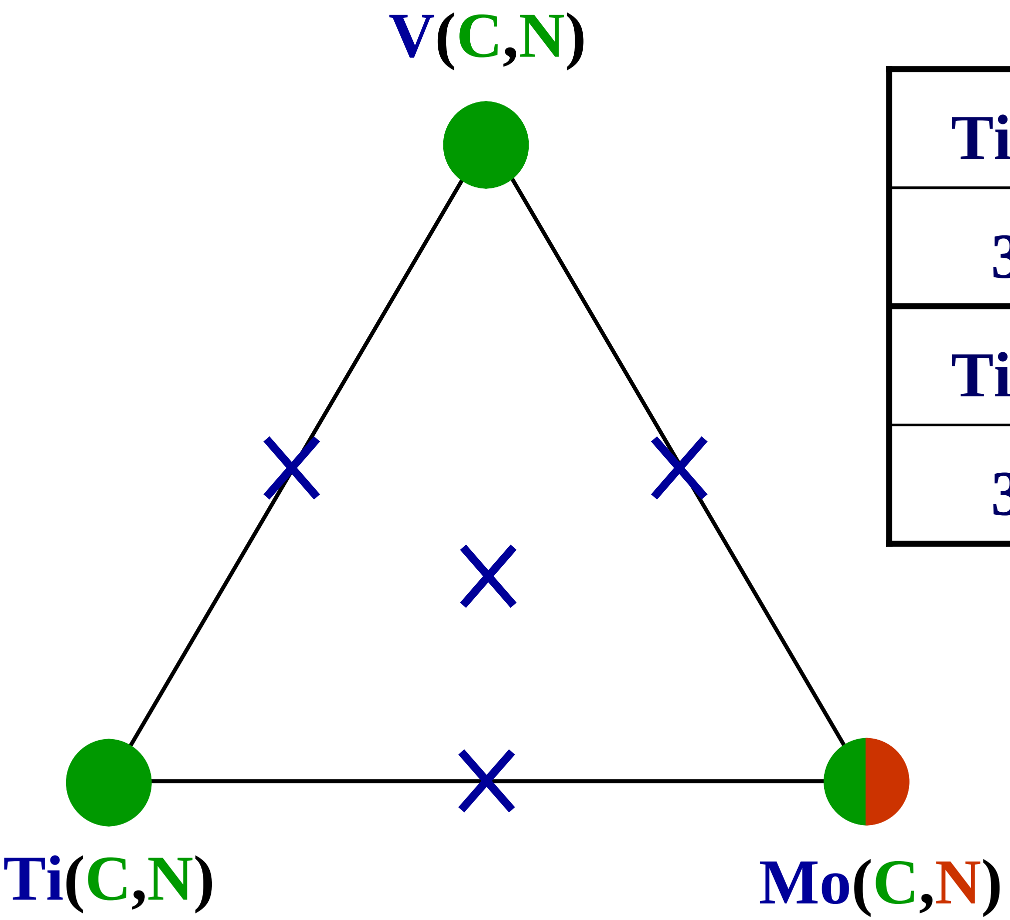
  Fe-C : 0.12 e/(a.u.)^3 Fe-N : 0.12 e/(a.u.)^3

(cf) 1 a.u.=0.529 Å

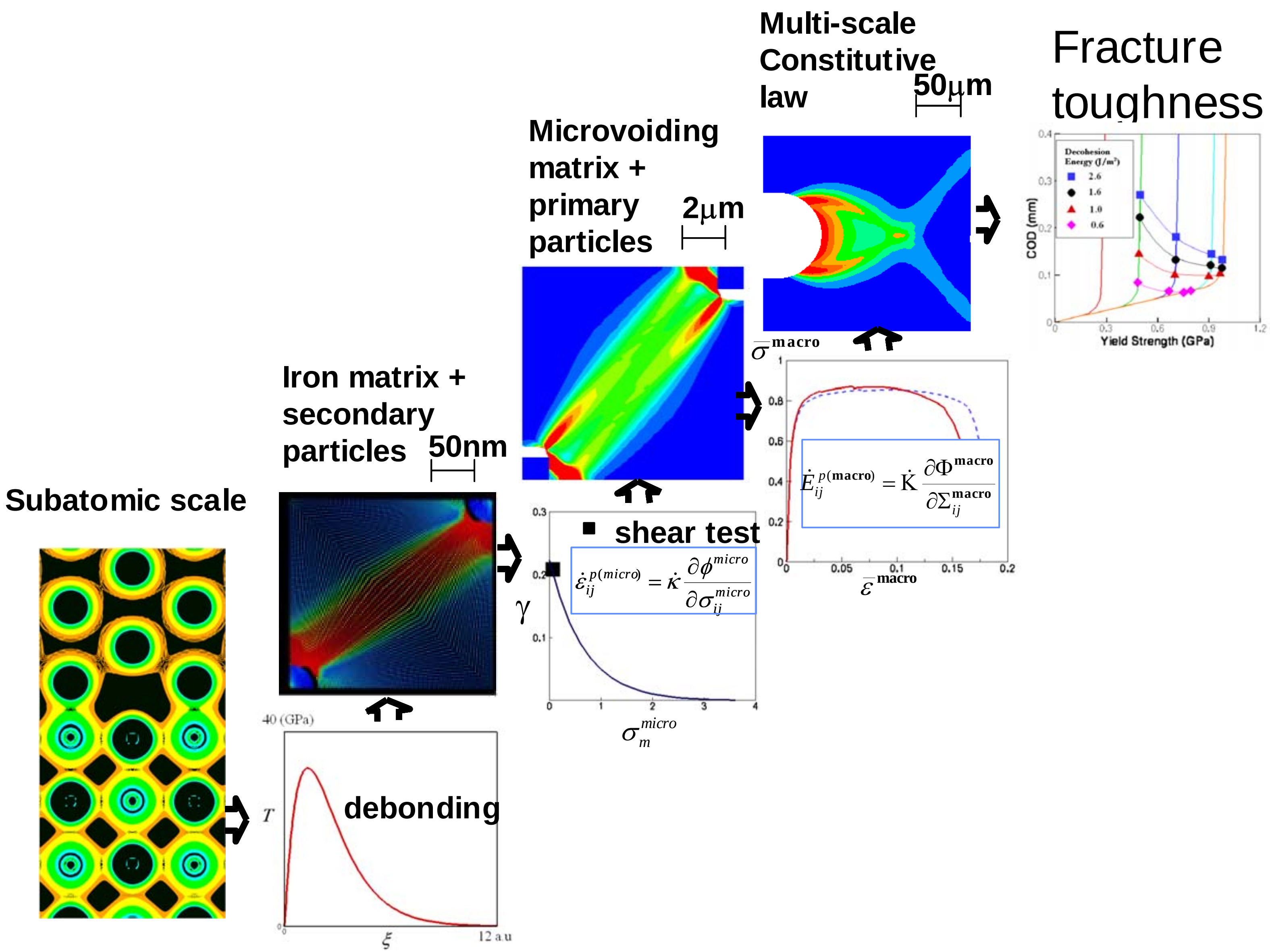
Interfacial Quantum Engineering of Grain Refining Carbonitrides

MX/Fe

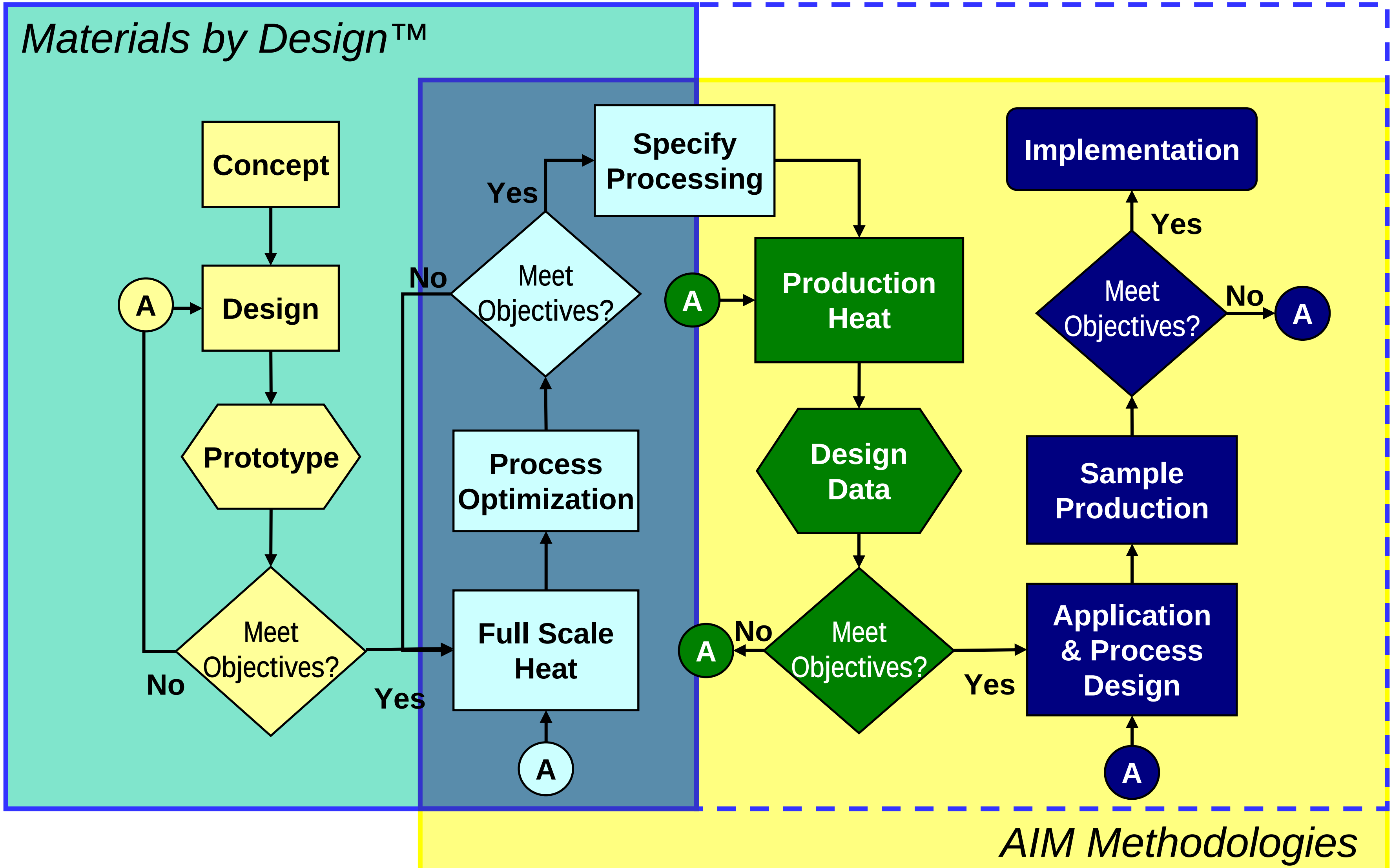
Work of Separation (J/m²)



TiC/Fe	VC/Fe	MoC/Fe
3.89	3.70	3.46
TiN/Fe	VN/Fe	MoN/Fe
3.29	3.17	4.31


Subatomic scale
Iron matrix + secondary particles
50nm
debonding
40 (GPa)
T
ξ
12 a.u
Microvoiding matrix + primary particles
2μm
shear test
γ
$\dot{\varepsilon}_{ij}^{p(micro)} = \dot{\kappa}\frac{\partial\phi^{micro}}{\partial\sigma_{ij}^{micro}}$
σ_m^{micro}
Multi-scale Constitutive law
50μm
$\bar{\sigma}^{macro}$
$\dot{E}_{ij}^{p(macro)} = \dot{K}\frac{\partial\Phi^{macro}}{\partial\Sigma_{ij}^{macro}}$
$\bar{\varepsilon}^{macro}$
Fracture toughness
Decohesion Energy (J/m²)
2.6
1.6
1.0
0.6
COD (mm)
Yield Strength (GPa)

Materials Development Cycle



AIM ARCHITECTURE

Integration Infrastructure

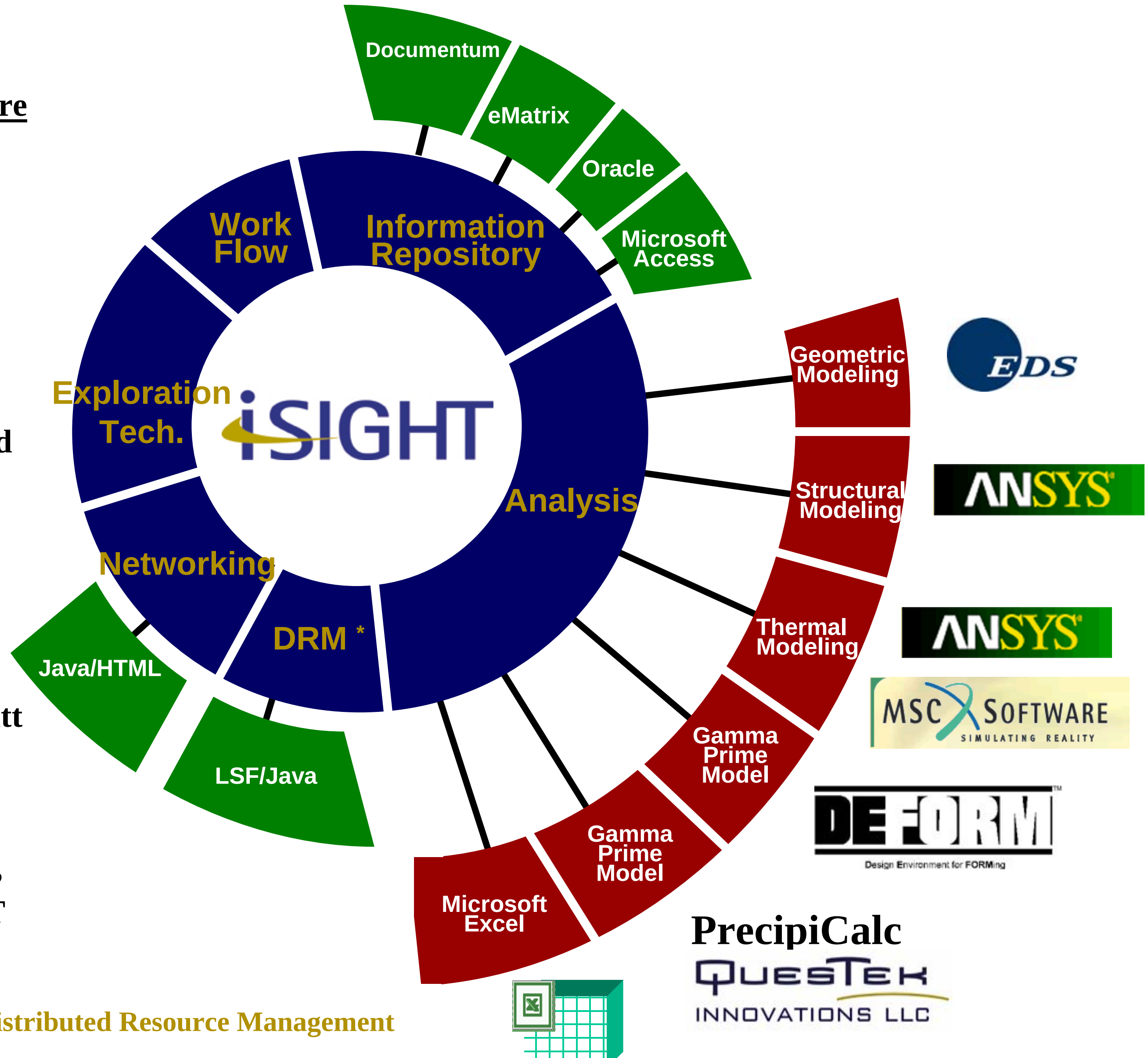
iSIGHT framework provided by Engineous Software

Core Utilities

3RD Party tools to extend iSIGHT's integration capabilities

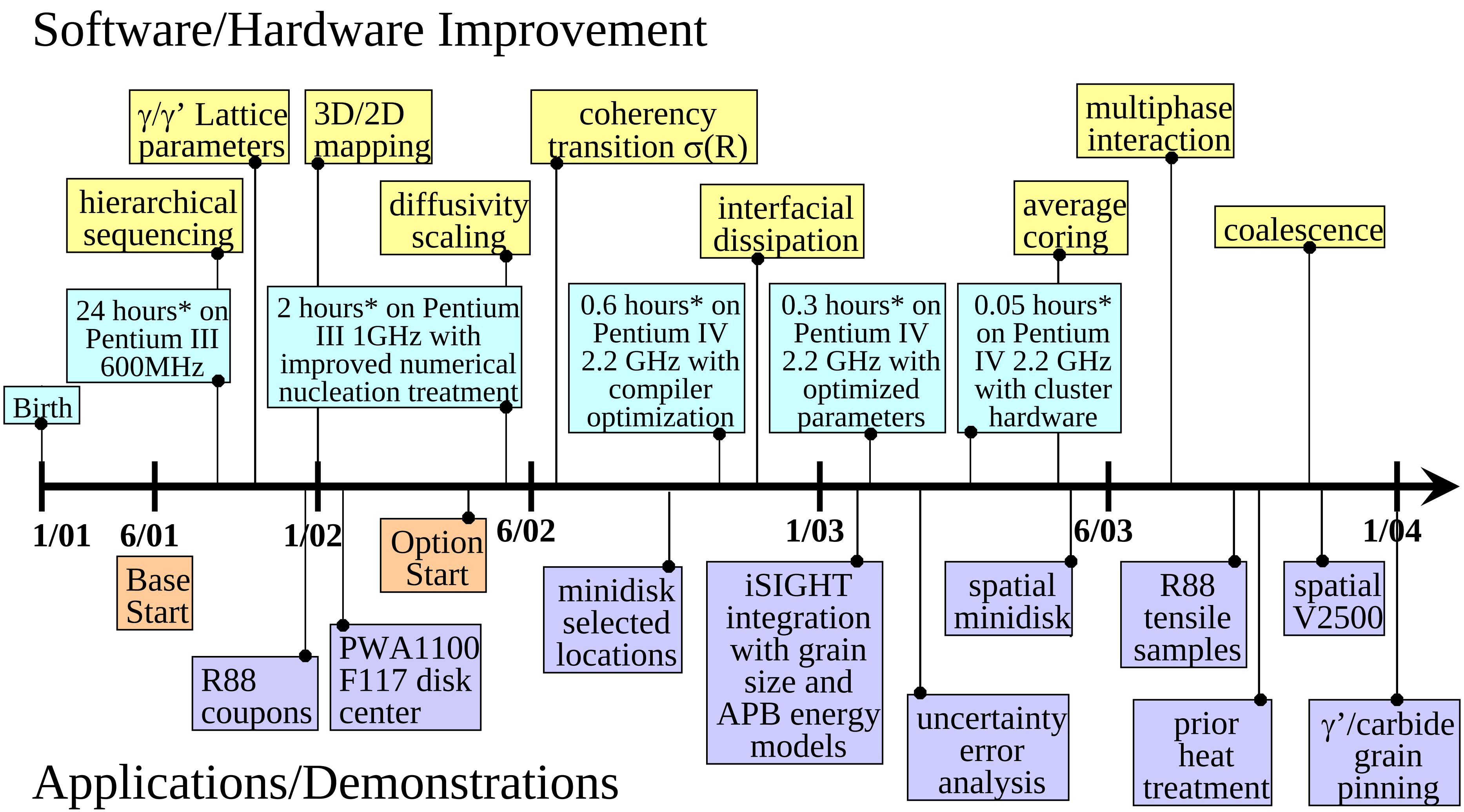
Analysis Components

Models provided by Pratt & Whitney, General Electric, Questek, and others. Integrated by Engineous into the DKB architecture via iSIGHT



* Distributed Resource Management

PrecipiCalc™ Timeline



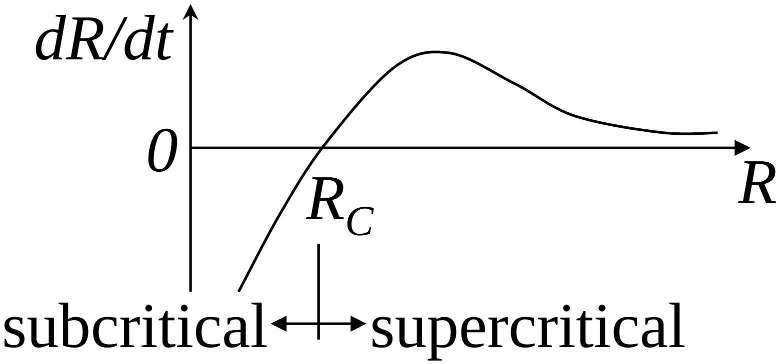
* single IN100 PWA1100 simulation

Basic *PrecipiCalc* Equations (2) — Particle Growth

$$\text{Growth}: \frac{dR}{dt} = \frac{\left(1 + R\sqrt{4\pi N_v \langle R \rangle}\right)}{\left(R\Gamma + s(R) \Big/ \left(M_0 \exp\frac{-Q}{RT}\right)\right)} \left\{ \Delta G_m - \frac{2\sigma(R)\overline{V}_m^{\beta}}{R} \right\}$$

$$\text{where } \Delta G_m = \left[\overline{\Delta C_i}\right]^T \left[\frac{\partial^2 \overline{G}^{\alpha}}{\partial C_i \partial C_j}\right] \left[\Delta C_j^{\infty}\right] + \left[\overline{C}_m^{\beta}\right] \bullet \left(\left[\overline{\mu}_m^{\alpha}\right] - \left[\overline{\mu}_m^{\beta}\right]\right)$$

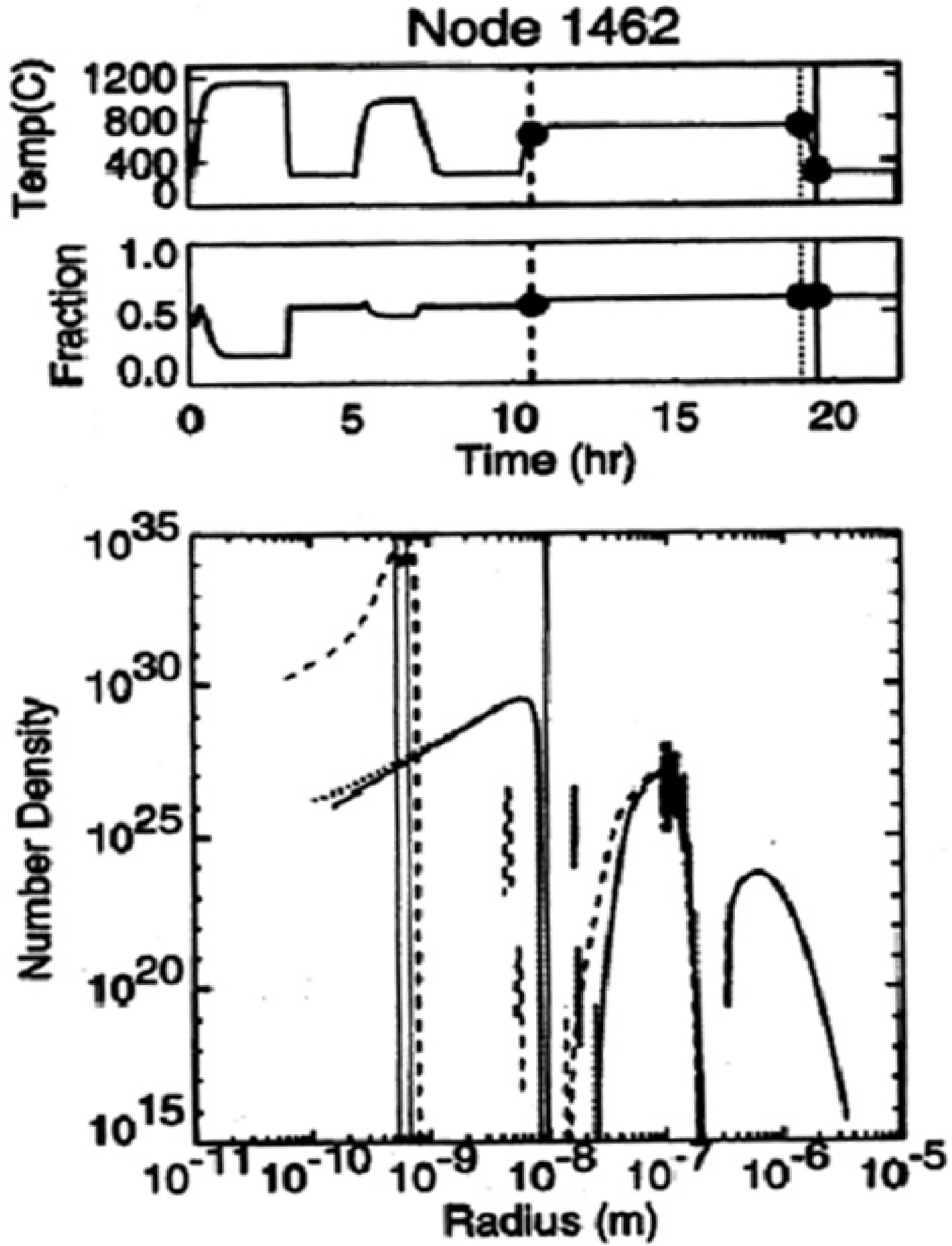
$$\Gamma = \left[\overline{\Delta C_i}\right]^T \left[\frac{\partial^2 \overline{G}^{\alpha}}{\partial C_i \partial C_j}\right] \left[\overline{D}_{jk}\right]^{-1} \left[\Delta C_k^{e}\right]$$



Thermodynamics

Diffusivity

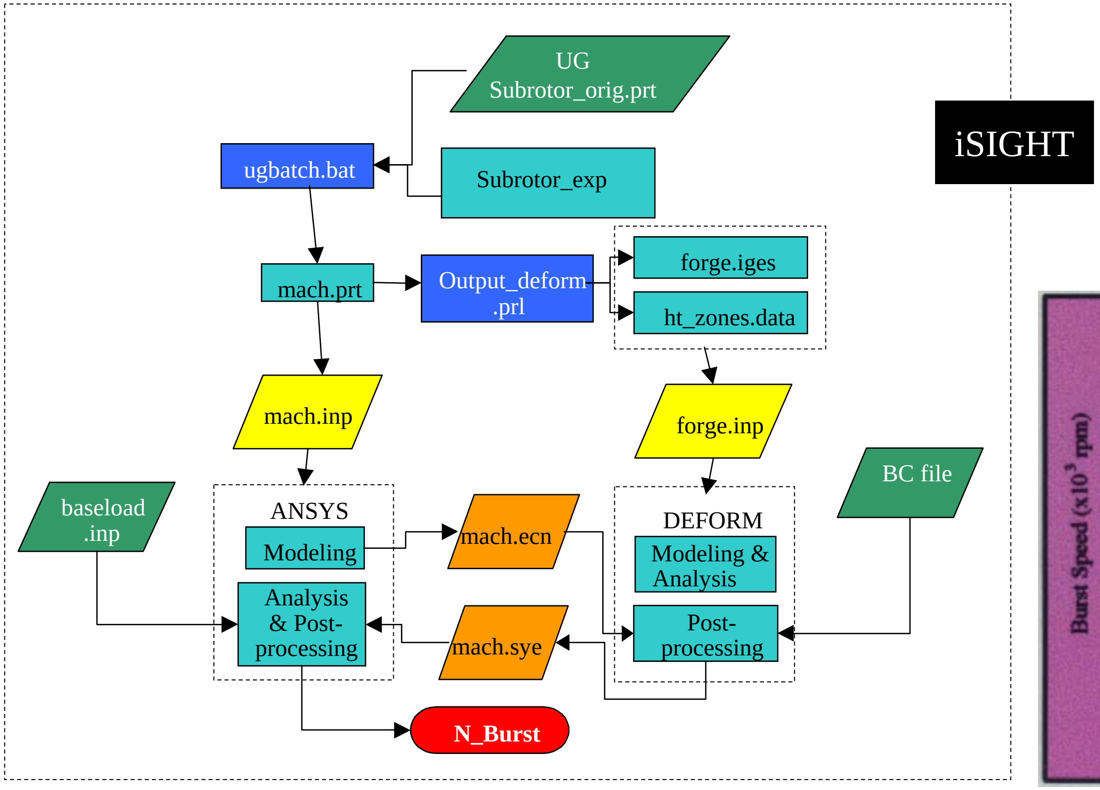
Interfacial Property

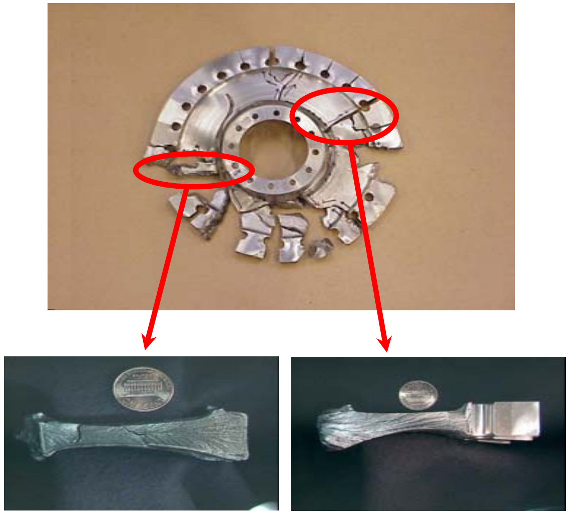


Node 1462
Temp(C)
1200
800
400
0
Fraction
1.0
0.5
0.0
0
5
10
15
20
Time (hr)
Number Density
10^{35}
10^{30}
10^{25}
10^{20}
10^{15}
10^{-11}
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
Radius (m)

Impact of DARPA AIM Initiative

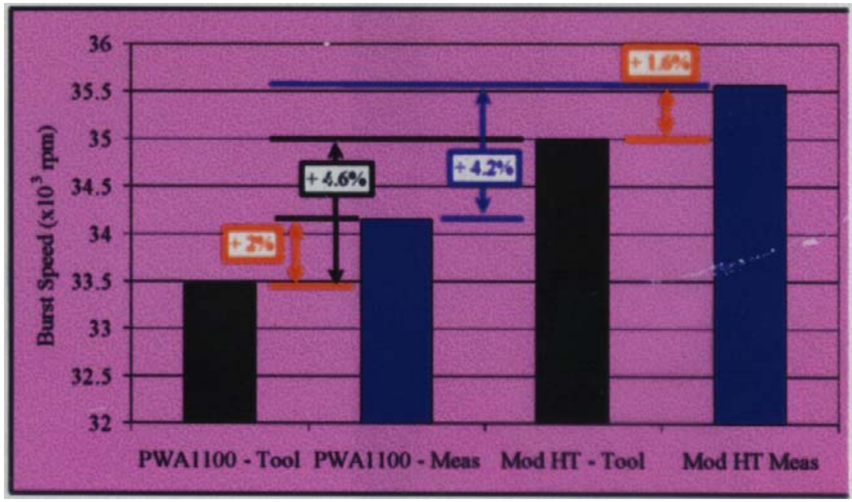
- Material behavior intimately linked and particpiating in the design process
  - ➢ 4 months to improved capability



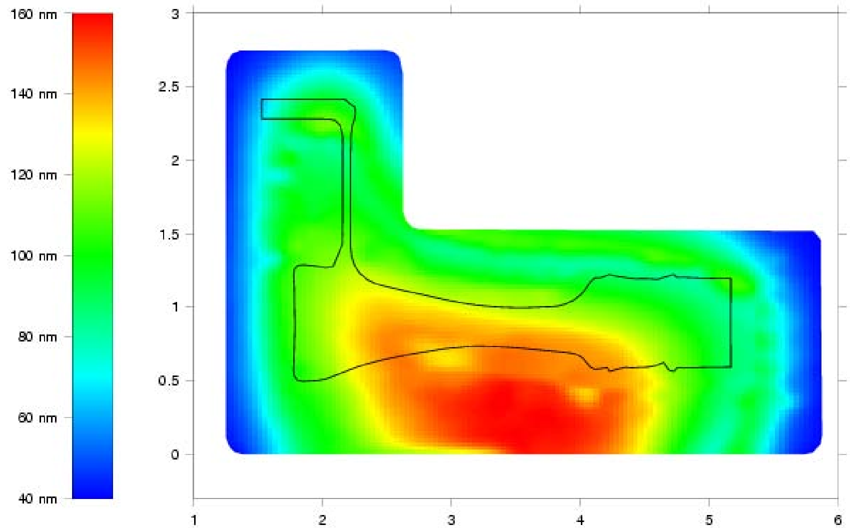


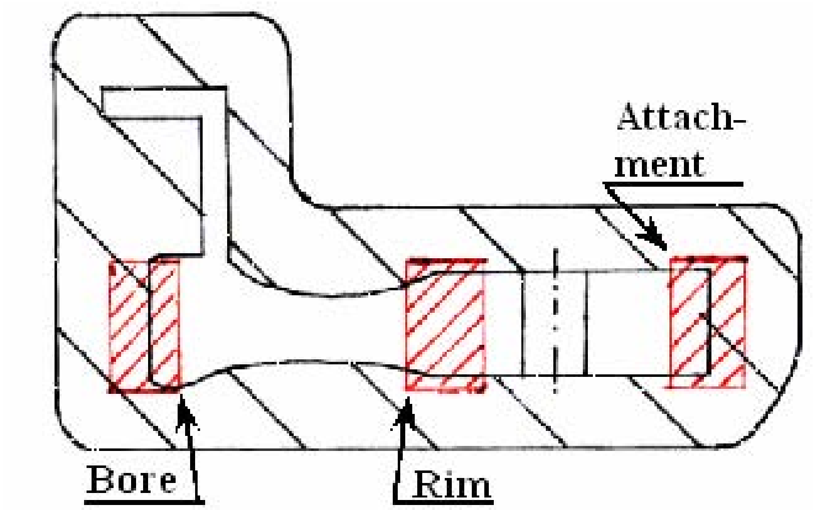
Rim hole

Bore



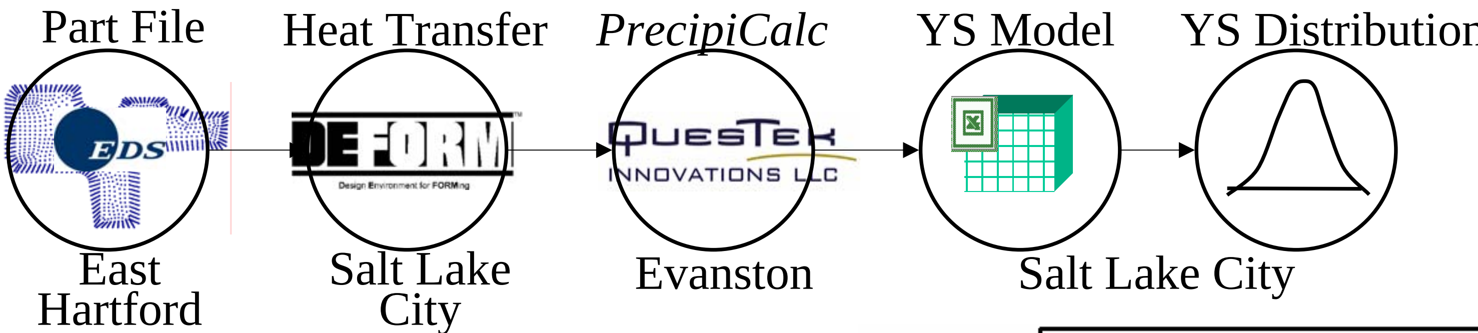
Minidisk Microstructure Prediction with *PrecipiCalc*



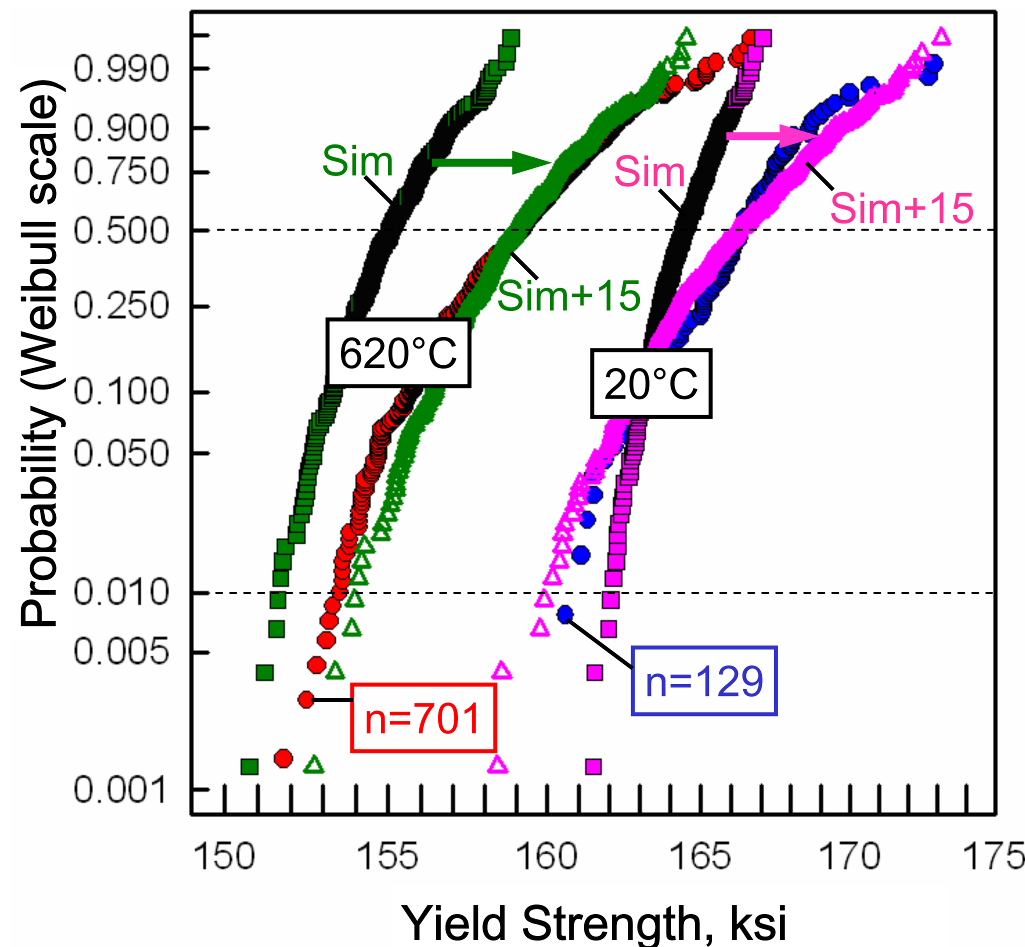


Minidisk Comparison		Bore		Rim		Attachment	
		Exp.	PpC	Exp.	PpC	Exp.	PpC
Primary γ’	Fraction (%)	24 25.2	22.6	23.5 25	23.5	23.1 25.7	23.3
	Size (μm)	1.28	1.29	1.23 1.27	1.32	1.18 1.2	1.31
Secondary γ	Fraction (%)	32.4	35		34		34.6
	Size (nm)	109 129	107.9	132 157	120 135 146	103 114	84.2
Tertiary γ’	Size (nm)	18 20.8	21.5	19.7 21.8	21.4	21.4	20.7

Probabilistic Modeling of Manufacturing Variation: PrecipiCalc™ Forecast of Minimum Design Properties



Mechanistic simulation + (n=15) gives good prediction of 1% minimum YS.



ACCELERATING TECHNOLOGY TRANSITION
Bridging the Valley of Death for Materials and Processes in Defense Systems

Committee on Accelerating Technology Transition
National Materials Advisory Board
Board on Manufacturing and Engineering Design
Division on Engineering and Physical Sciences

NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

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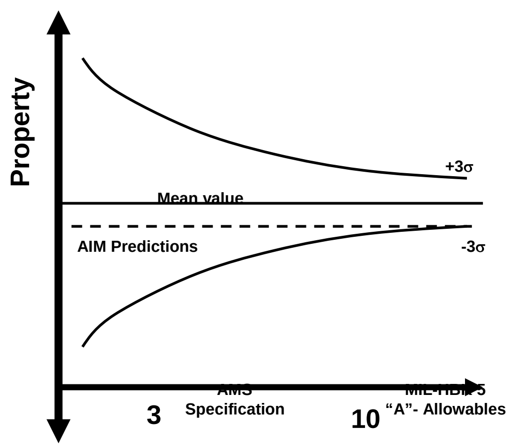
Washington, D.C.
www.nap.edu

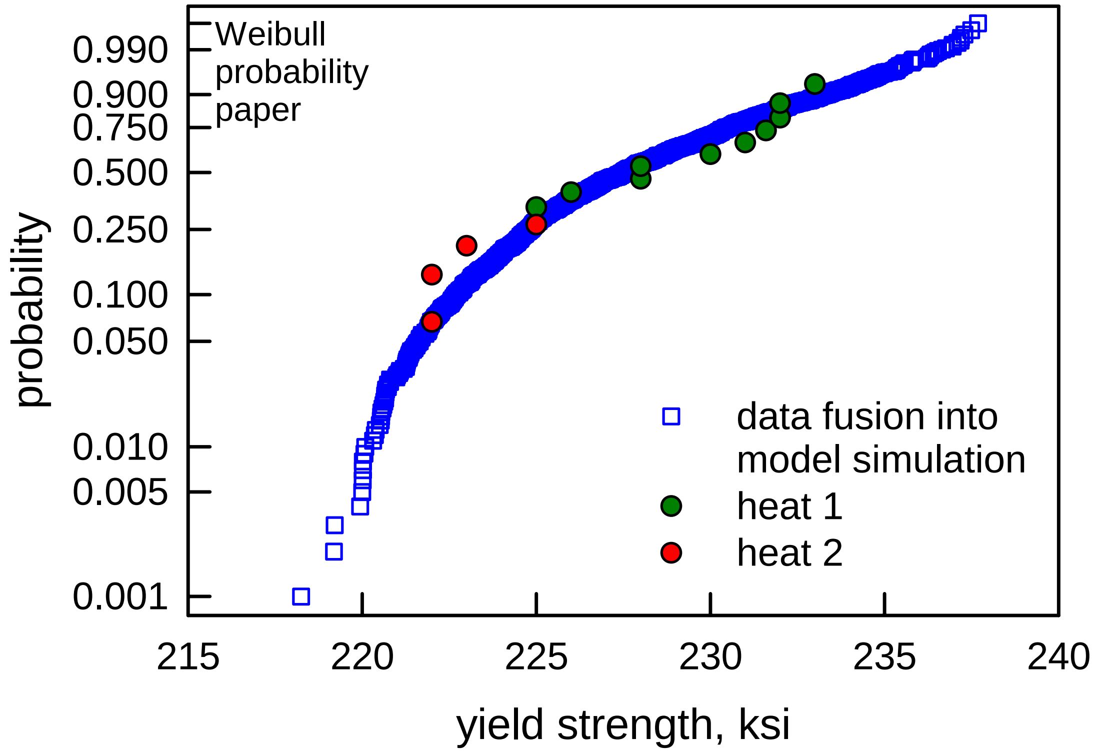
TABLE 3.1 Some Computational Materials Engineering Tools

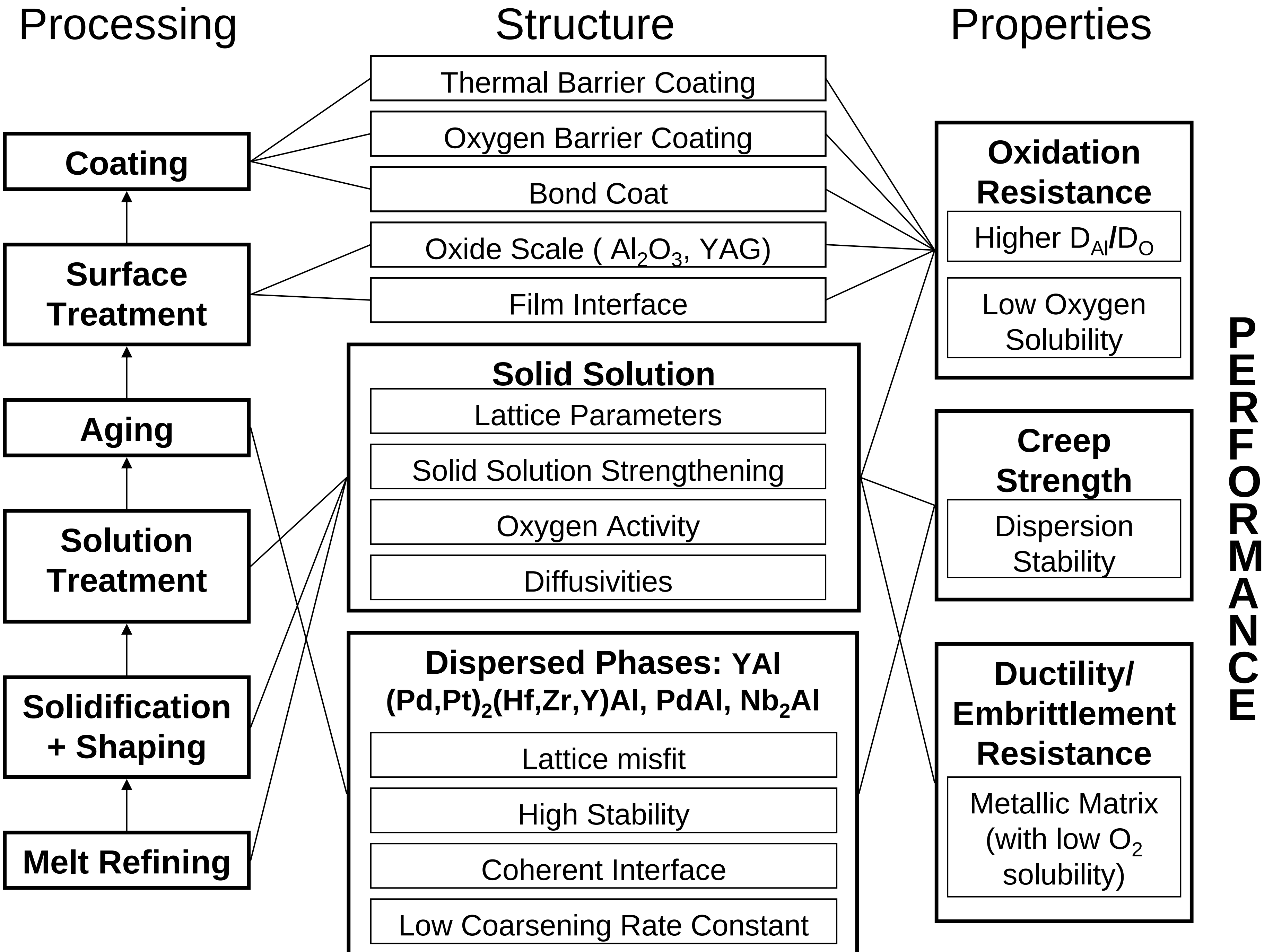
Type	Tool	Company	Function
Design integration	iSIGHT	Engineous Software (Salt Lake City, Utah)	Multidisciplinary design optimization (MDO)
	CMD	QuesTek Innovations LLC (Evanston, Illinois)	Parametric materials design
Macroscopic process modeling	ProCAST	ESI Group (Paris, France)	Solidification processing
	DEFORM-HT	Scientific Forming Technologies Corporation (Columbus, Ohio)	Deformation processing and heat transfer (finite-element method)
Microstructural simulation	PrecipiCalc	QuesTek Innovations LLC (Evanston, Illinois)	High-fidelity precipitation simulation
	DICTRA	ThermoCalc AB (Stockholm, Sweden)	Multicomponent diffusion
	J MatPro	Thermotech Ltd. (Surrey, United Kingdom)	Phase relations and basic microstructural modeling
Thermodynamics	ThermoCalc	ThermoCalc AB (Stockholm, Sweden)	Multicomponent thermodynamics and phase diagrams
	Pandat	CompuTherm LLC (Madison, Wisconsin)	Multicomponent thermodynamics and phase diagrams
	FactSage	Thermfact CRCT (Montreal, Canada)	Multicomponent thermodynamics and phase diagrams

ESTCP AIM Demonstration

- **Objective is to predict MIL-HBK 5 “A”- Allowables with only 3 heats available.**

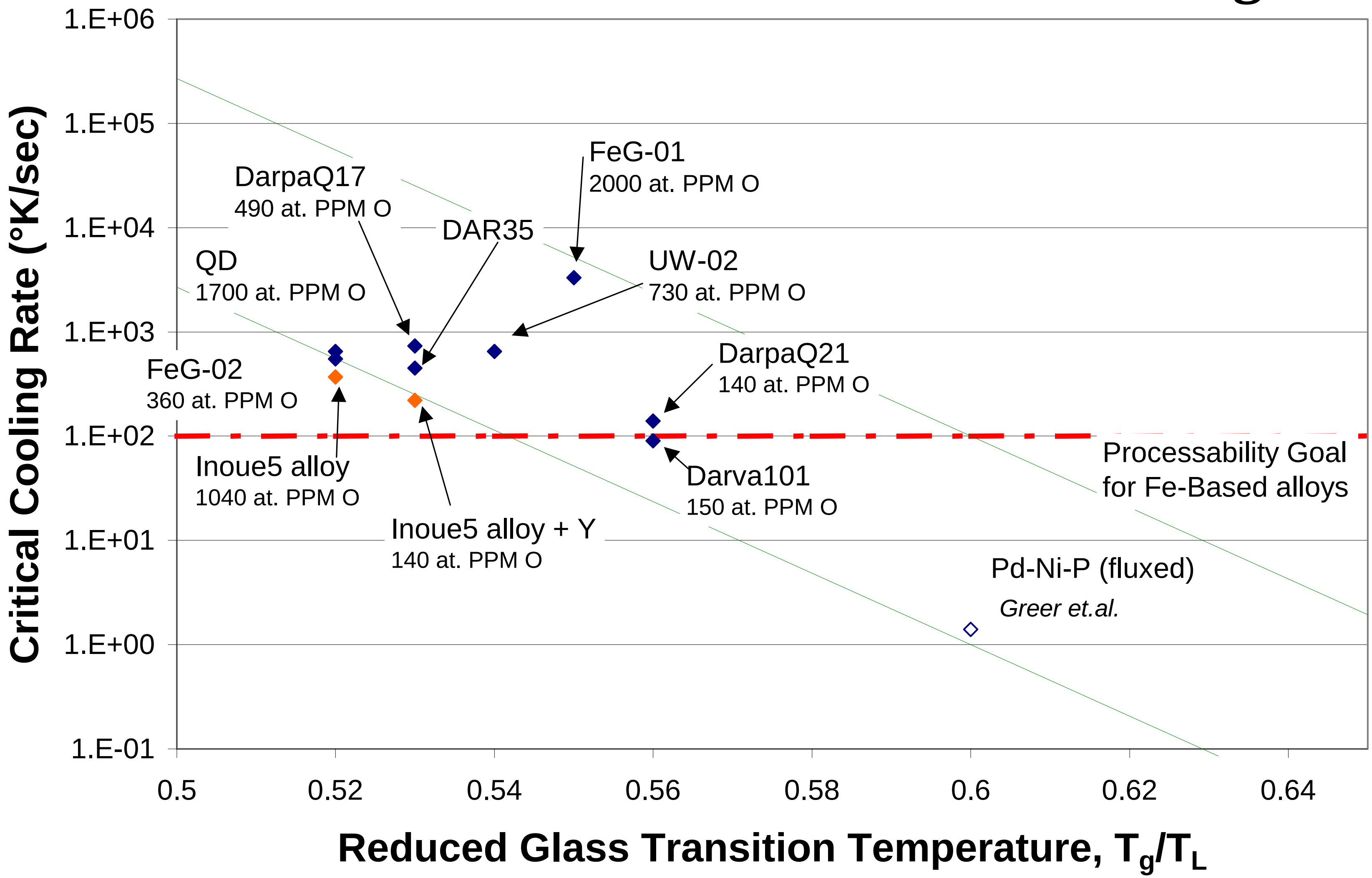






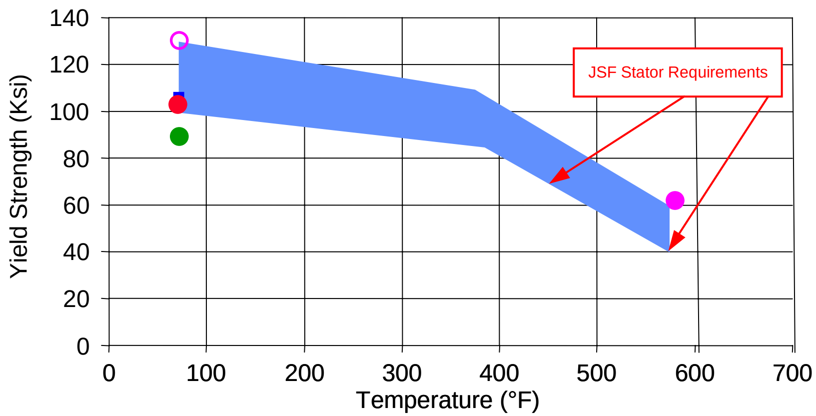
System chart

Critical Cooling Rate vs. T_{rg}

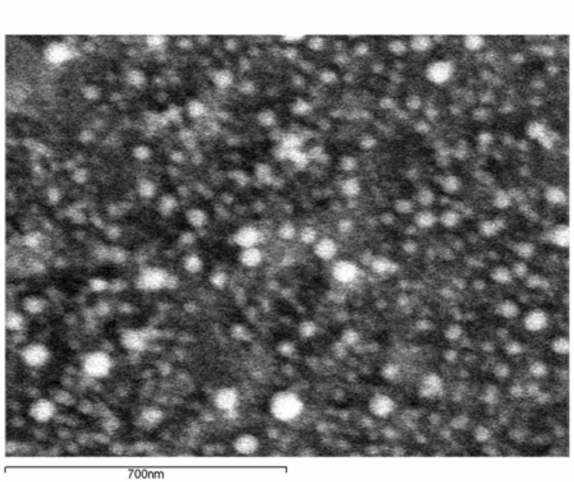


Twin-Roll Casting at IMI

High Temperature Aluminum by Glass Devitrification

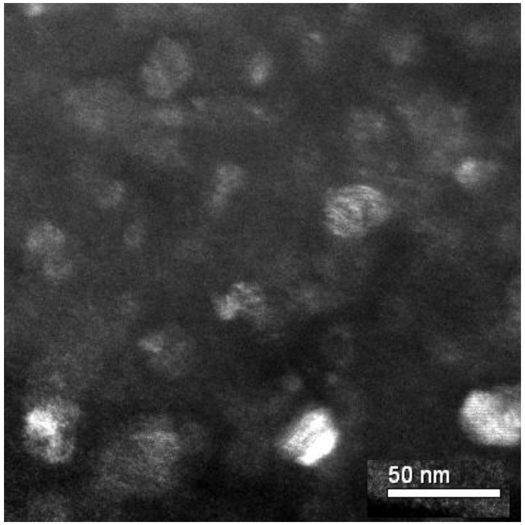


Bend test properties

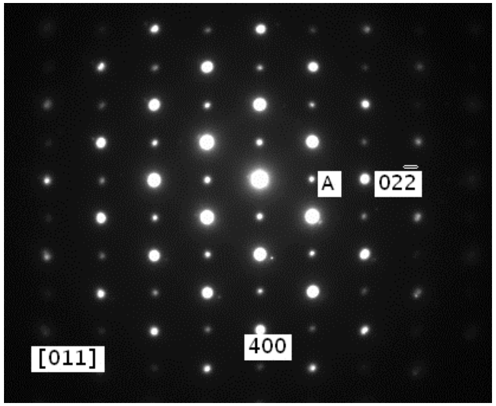


700nm

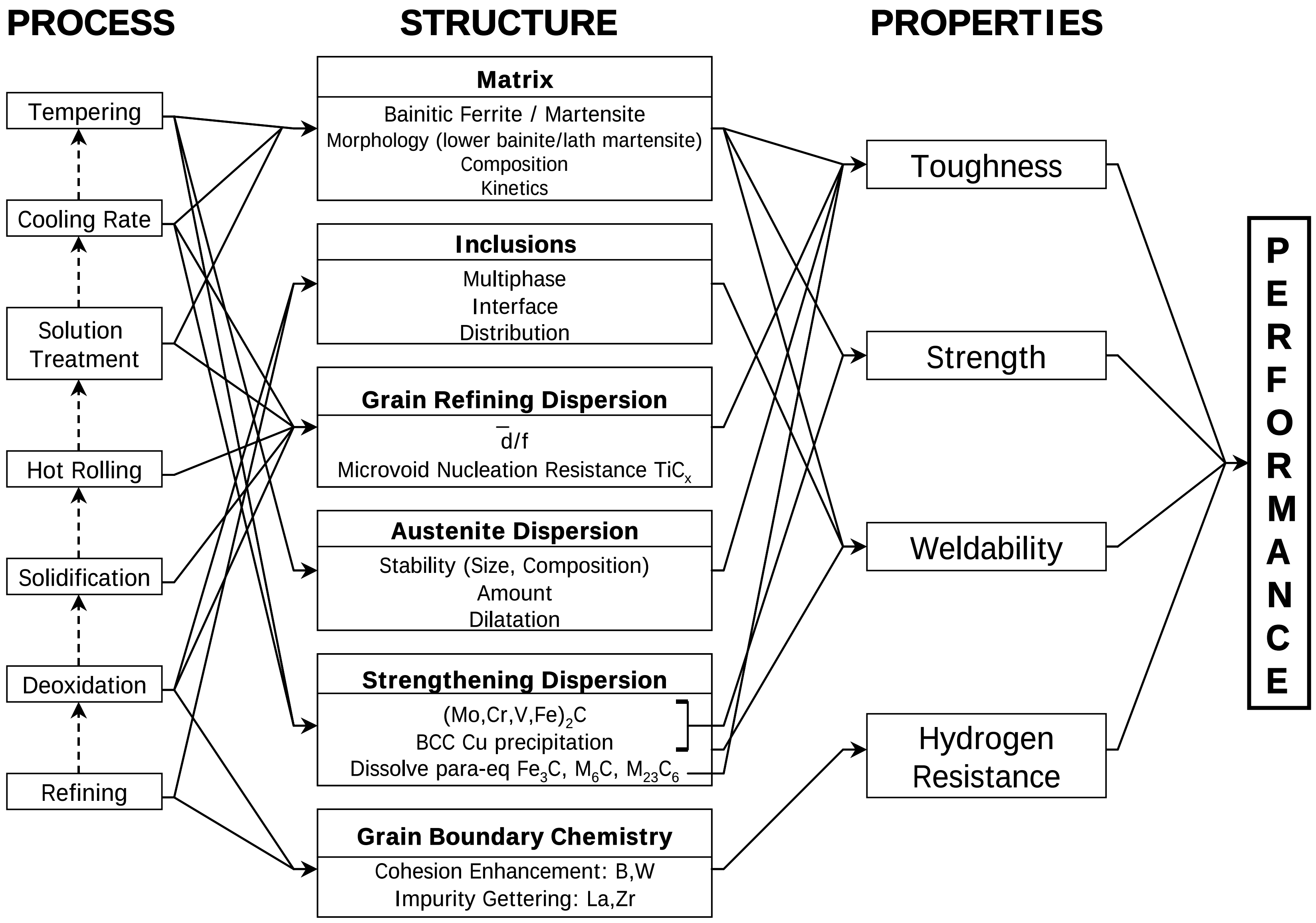
SEM image of $L1_2$ particle dispersion.



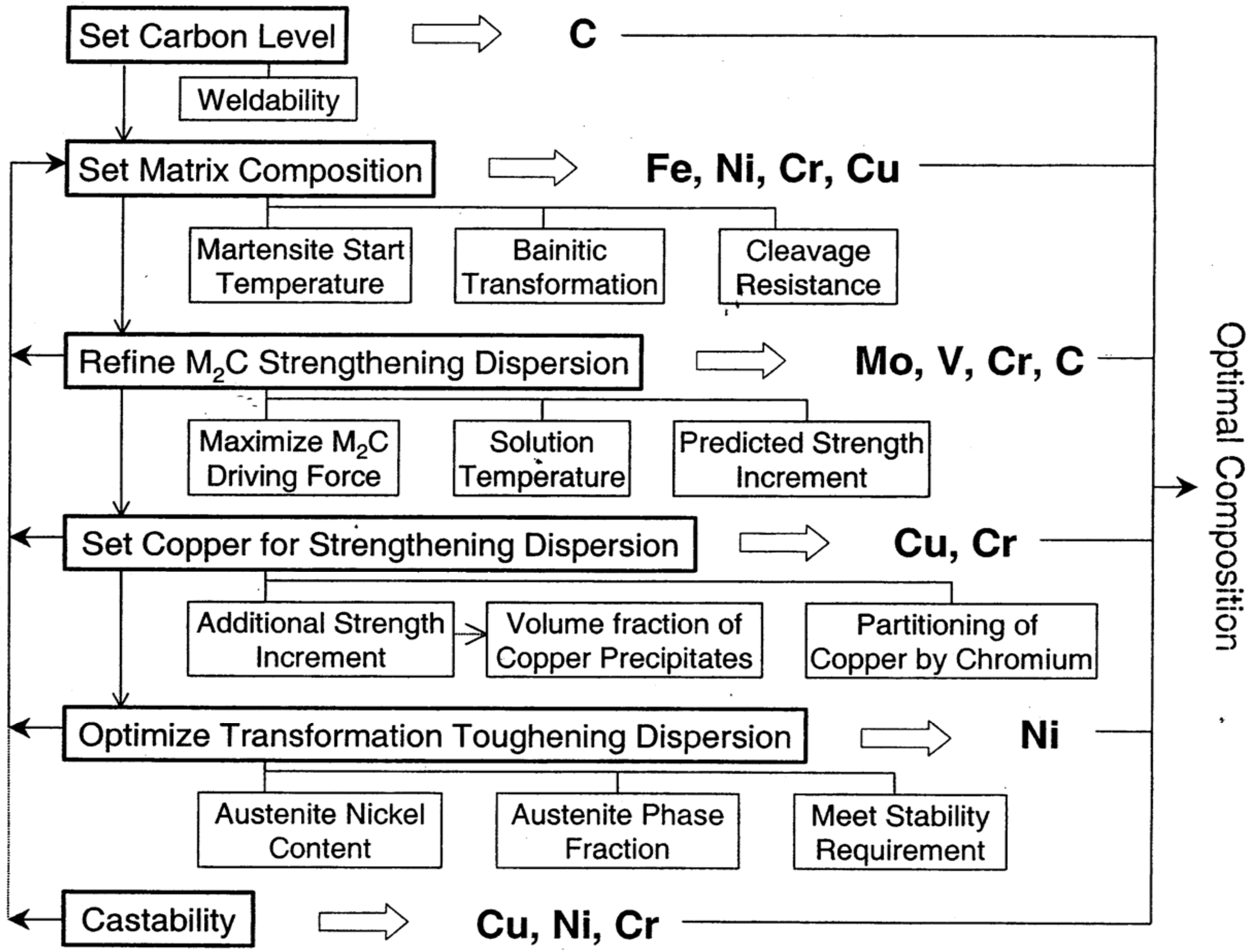
TEM Dark field image indicates $L1_2$ particles $\bar{d}$ ~25nm.



SAD pattern recorded along the [011] direction showing the matrix and the precipitates a cube/cube orientation relationship.

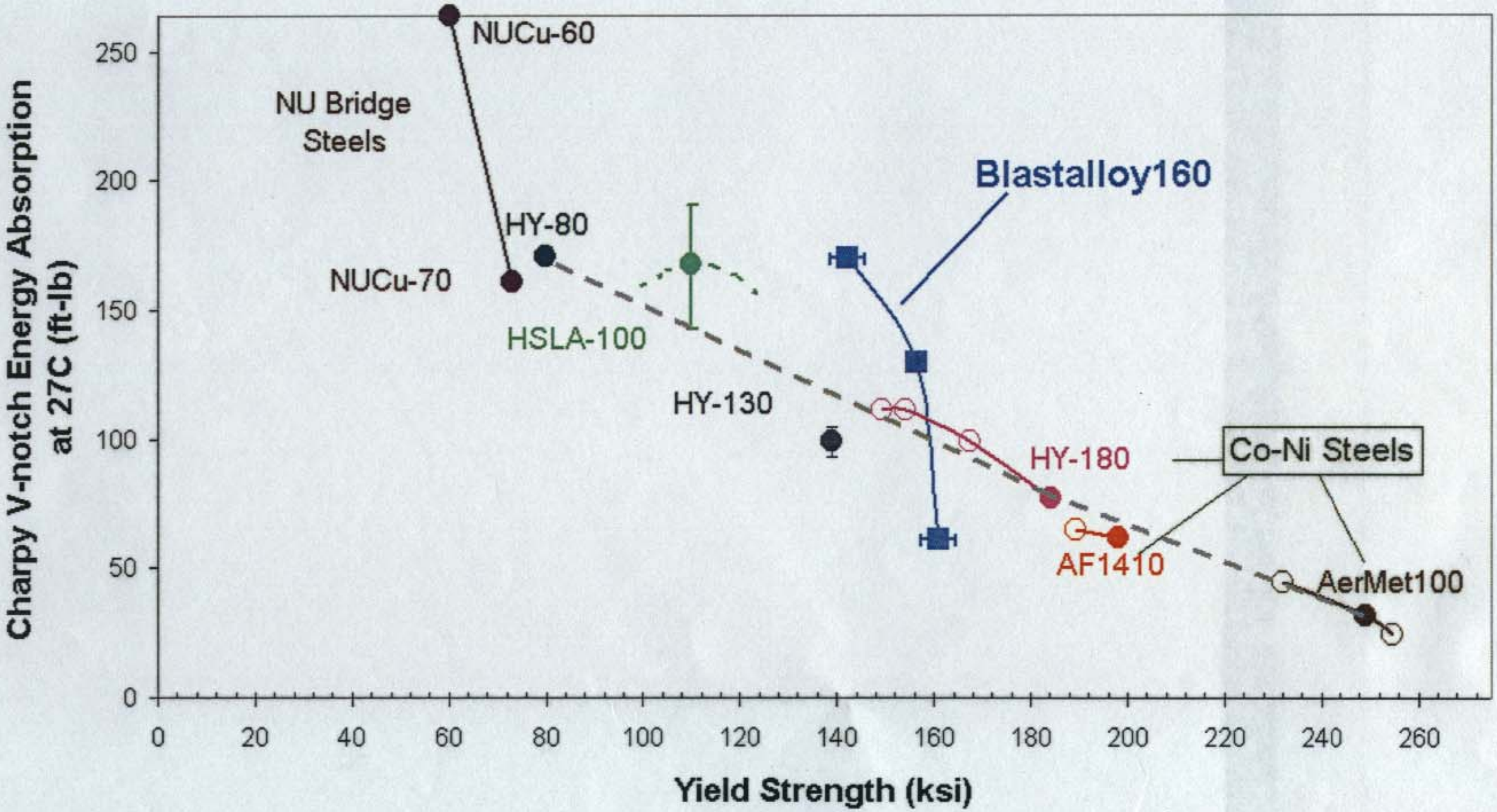


Systems Design Chart for Blast resistant Naval Steels



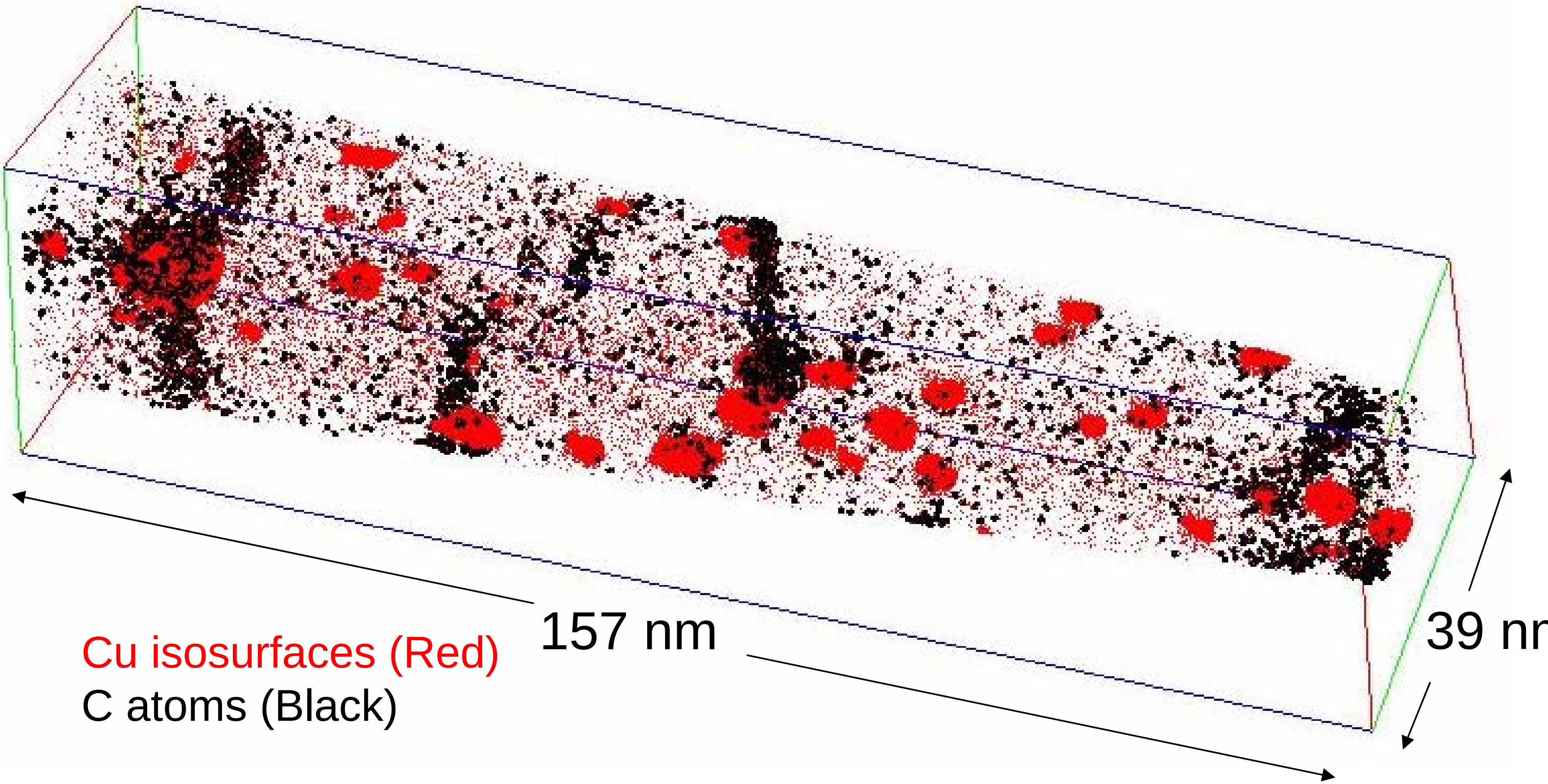
Optimal Composition

Toughness – Strength Combination

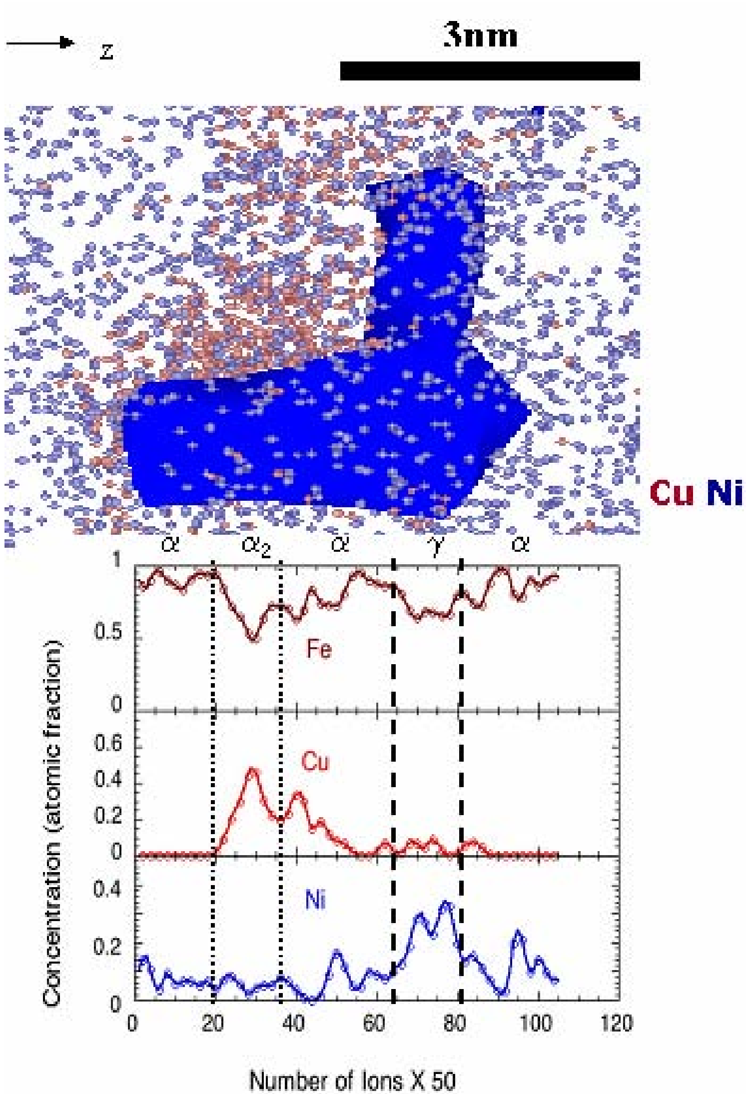


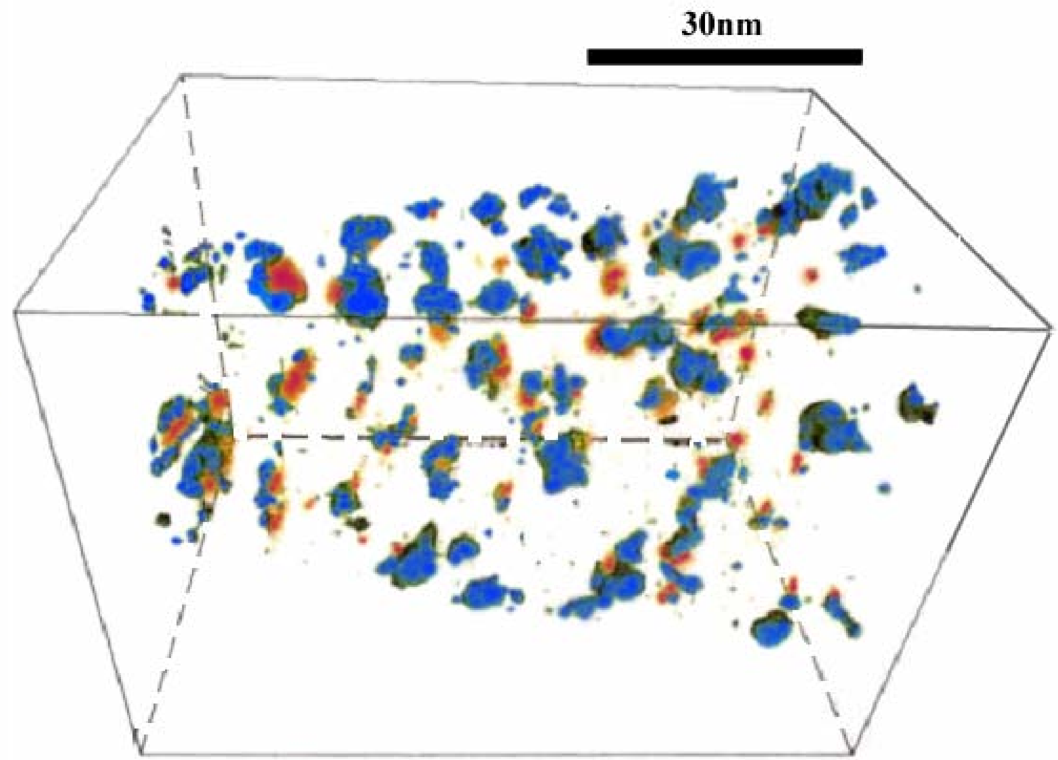
BA160 Alloy

39 x 39 x 157 nm^3 LEAP Reconstruction



Cu isosurfaces (Red)
C atoms (Black)

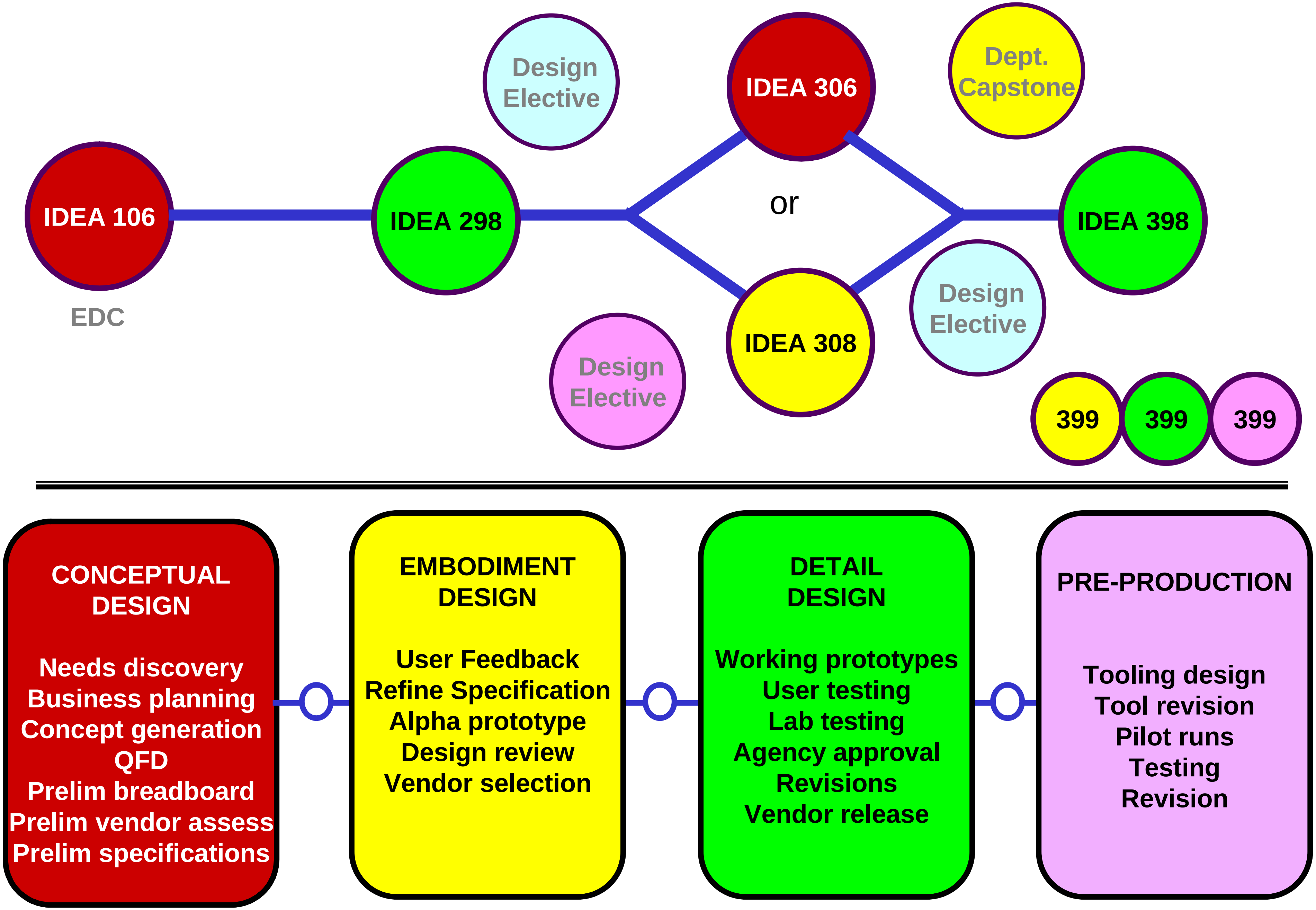

z
3nm
Cu Ni
α
α2
α
γ
α
Fe
Cu
Ni
Concentration (atomic fraction)
Number of Ions X 50


30nm

3-DAP

1. Scieneering Research
2. Techmanities Education

Design phases



Inspired by the HLB Process; courtesy Walter Herbst

MSC 390 Materials Design

Spring 2005

Design Projects

I. **Blastalloy 120 NM (396/EDC)**
Client: ONR, DHS
Advisors: Chris Kern, QuesTek
Padmanava Sadhukhan

II. **Windmill Steel C64**
Client: GE Power Generation
Advisor: Yana Qian

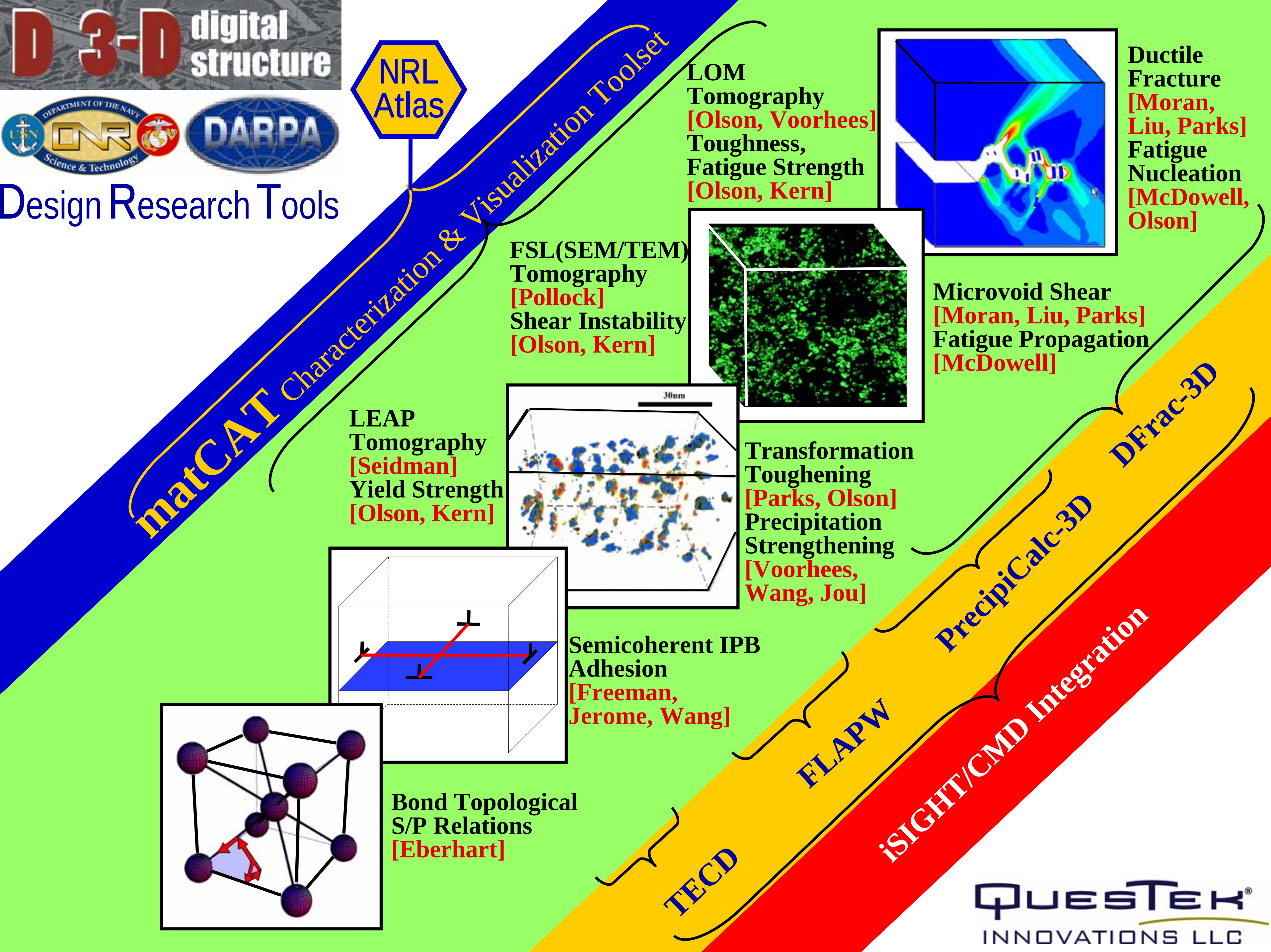
III. **NanoDie M60N**
Client: ITW Medalist
Advisor: Ben Tiemens

IV. **Terminator 4: Biomimetic Self-Healing Mg Composite**
Client: NASA, ARL
Advisor: Michele Manuel

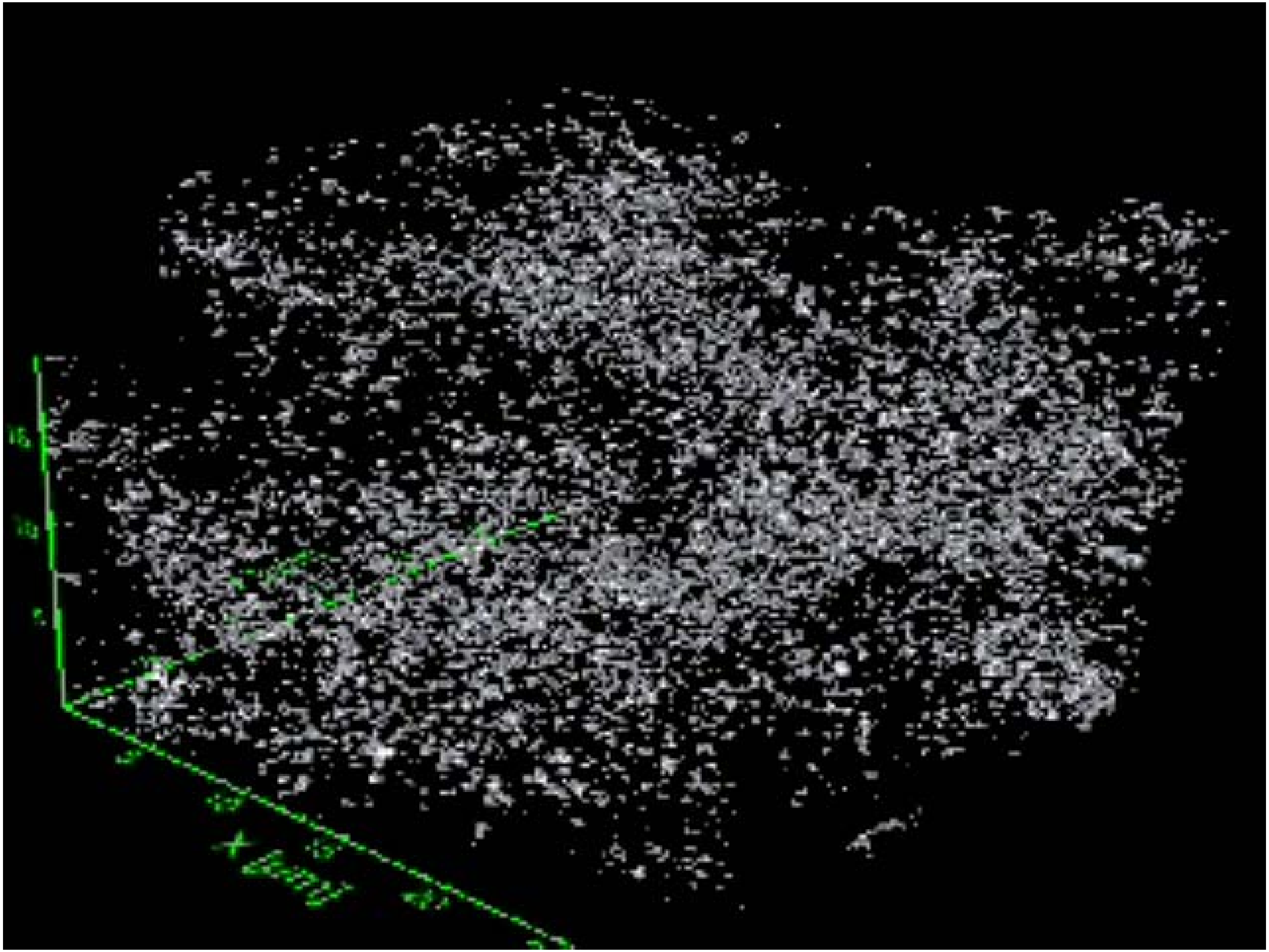
V. **Stentalloy Z: HP-SMA (396)**
Client: Medtronic, Memry
Advisor: Matt Bender

VI. **Noburnium 2: YAGalloy 1300**
Client: AFOSR, NASA, RMC
Advisor: Dave Bryan

VII. **Super Bubble (EDC)**
Client: QuesTek
Advisor: Les Morgret


D 3-D digital structure
DEPARTMENT OF THE NAVY
ONR
Science & Technology
DARPA
Design Research Tools
NRL Atlas
matCAT Characterization & Visualization Toolset
LOM
Tomography
[Olson, Voorhees]
Toughness,
Fatigue Strength
[Olson, Kern]
Ductile
Fracture
[Moran, Liu, Parks]
Fatigue
Nucleation
[McDowell, Olson]
FSL(SEM/TEM)
Tomography
[Pollock]
Shear Instability
[Olson, Kern]
Microvoid Shear
[Moran, Liu, Parks]
Fatigue Propagation
[McDowell]
LEAP
Tomography
[Seidman]
Yield Strength
[Olson, Kern]
30nm
Transformation
Toughening
[Parks, Olson]
Precipitation
Strengthening
[Voorhees, Wang, Jou]
Semicoherent IPB
Adhesion
[Freeman, Jerome, Wang]
Bond Topological
S/P Relations
[Eberhart]
DFrac-3D
PrecipiCalc-3D
FLAPW
TECD
iSIGHT/CMD Integration
QuesTek
INNOVATIONS LLC

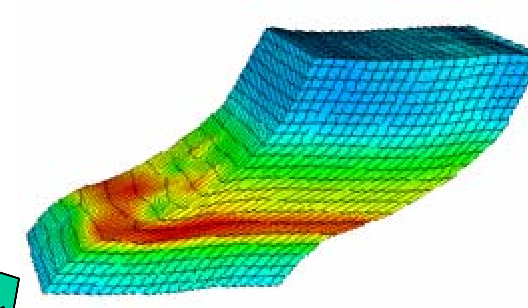
IN100 Alloy: Submicron Carbide Distribution



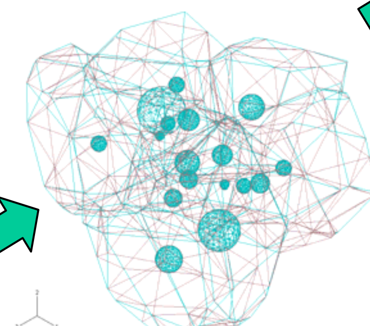
Shear Localization Simulation with Real Particle Clusters

Challenge Statement: Establish quantitative role of Particle dispersion nonuniformity in microvoid shear localization.

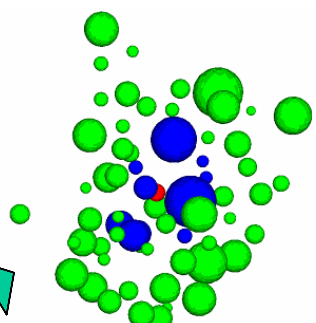
Approach: Analyze carbide dispersion nonuniformity in IN100 tomographic dataset and simulate shear localization at potent clusters embedded in steel matrix.



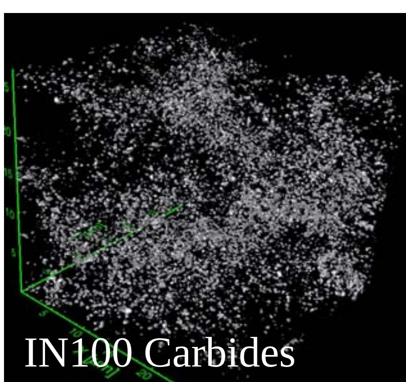
Shear Localization Simulation



3D Mesh

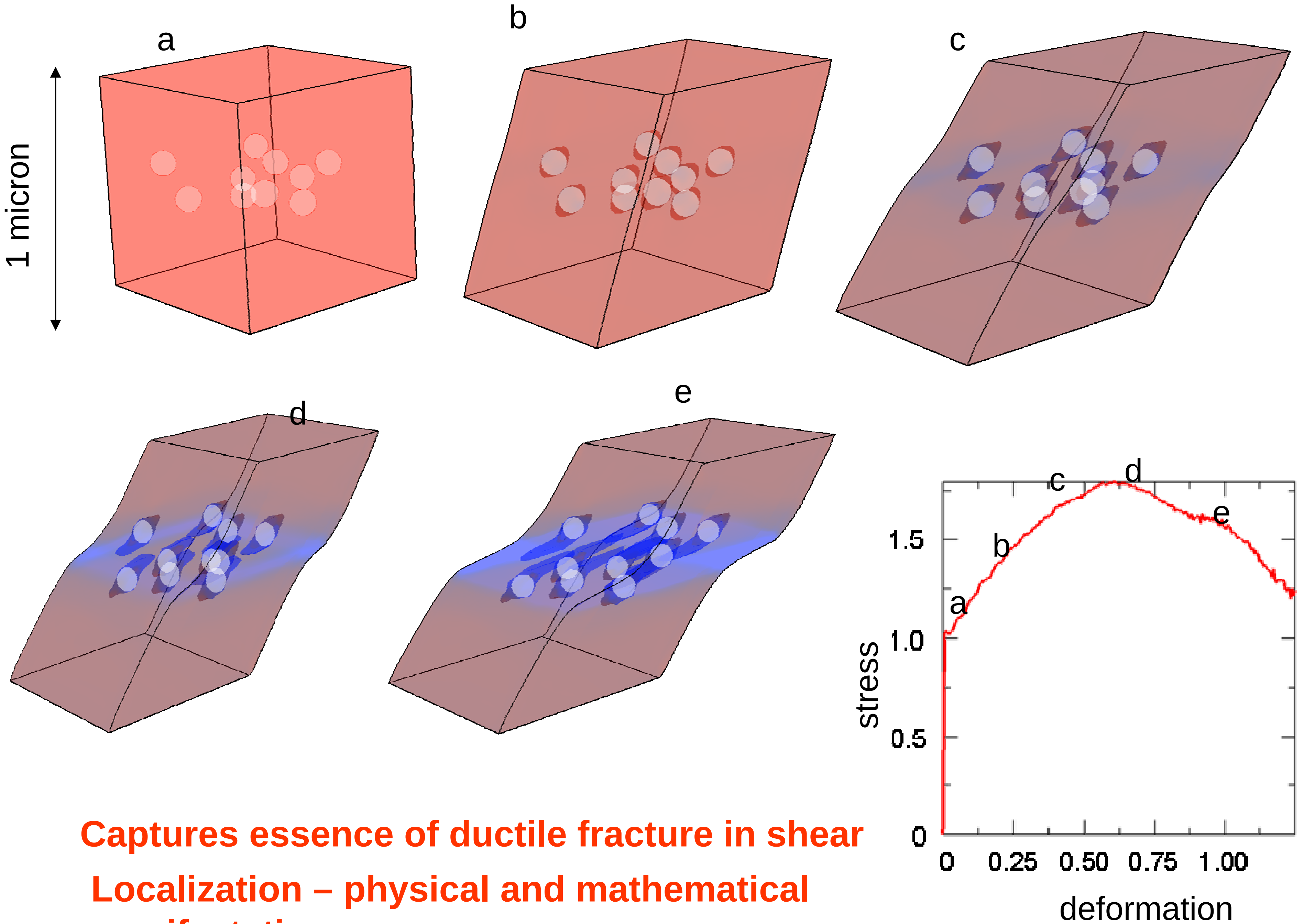


Identified Potent Cluster



Impact: Shear localization is of central importance in both fracture toughness and ballistic plugging resistance. Incorporation of design concepts in prototype steels already demonstrates improved ballistic FSP V50 (ONR Mantech).

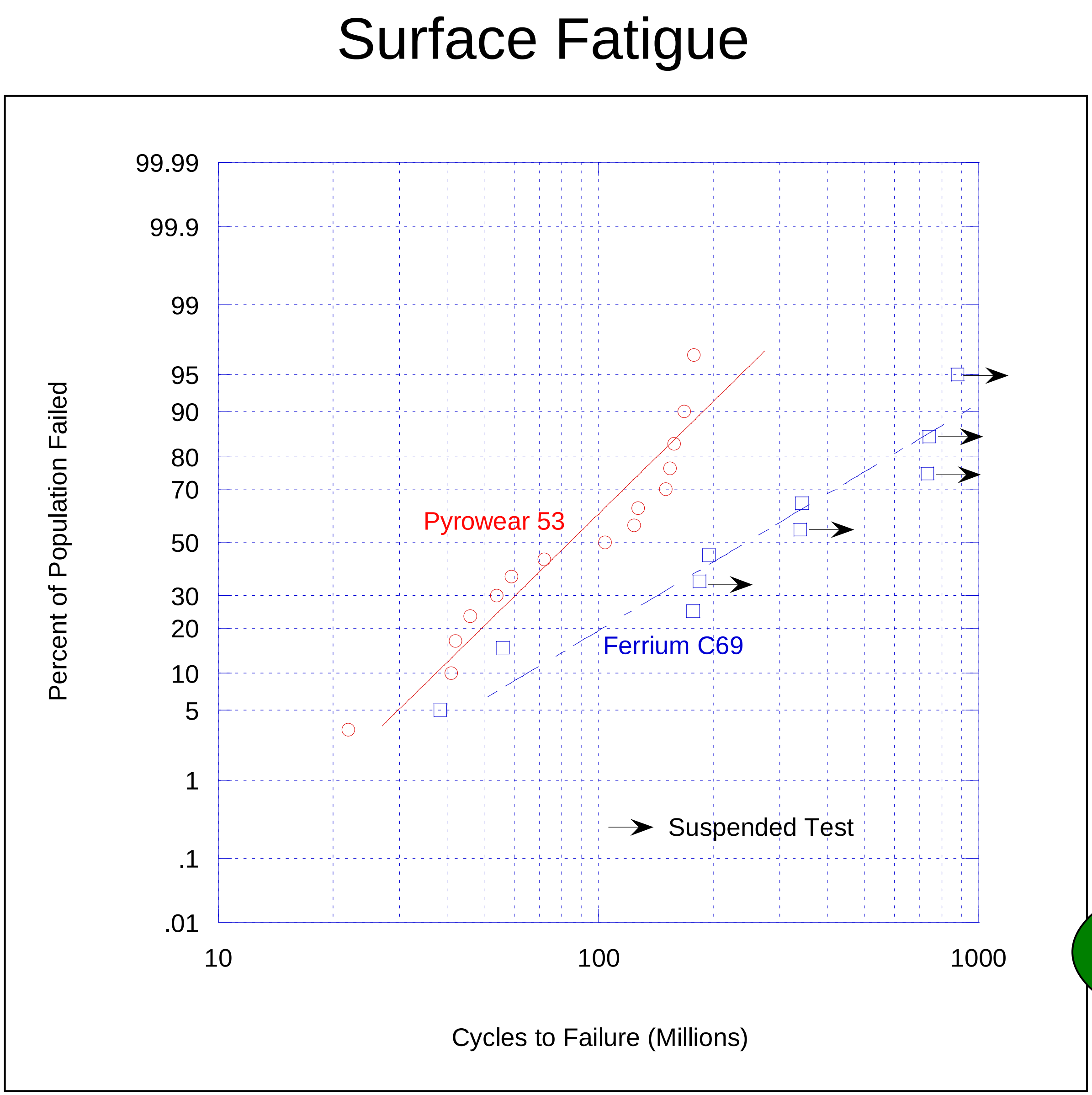
D.M. Parks, MIT, B. Moran, W-K. Liu Northwestern University; H.-J., QuesTek

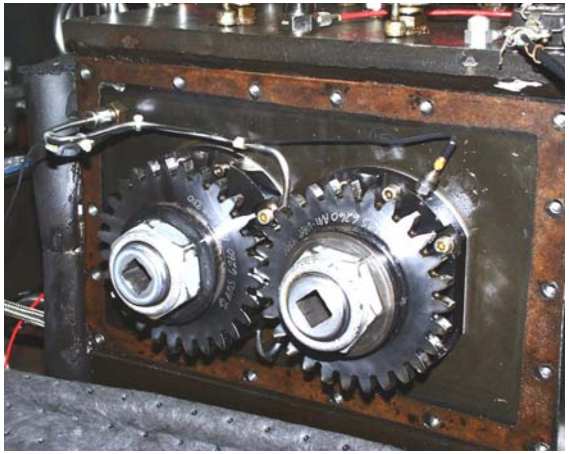


Captures essence of ductile fracture in shear

Localization – physical and mathematical manifestations

Ferrium C67- Performance

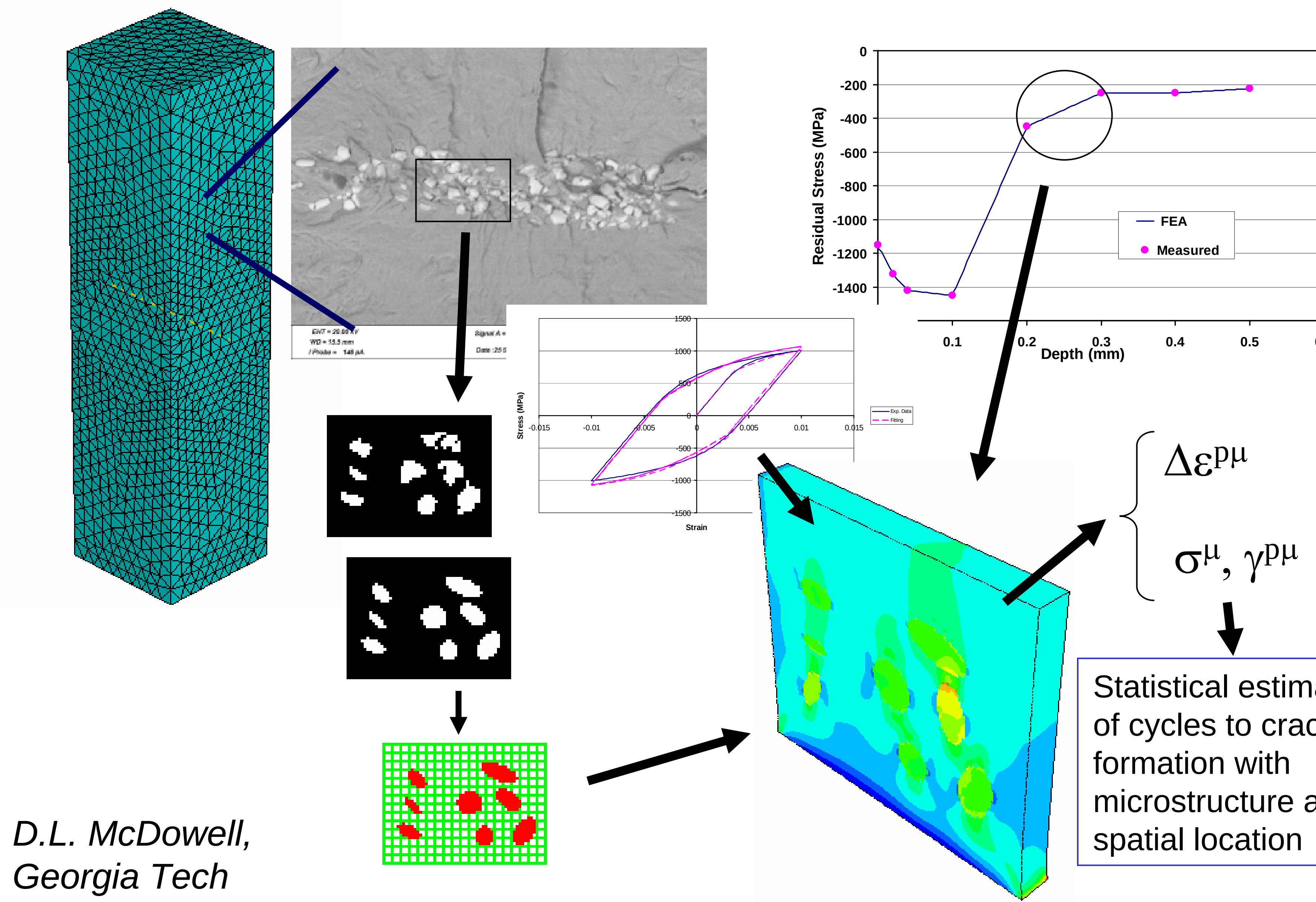




- NASA Glenn Research Center
- Recirculating Spur Gear Fatigue Rig
- Set to test surface fatigue, 1.72 GPa Hertzian stress

Best performing set to date

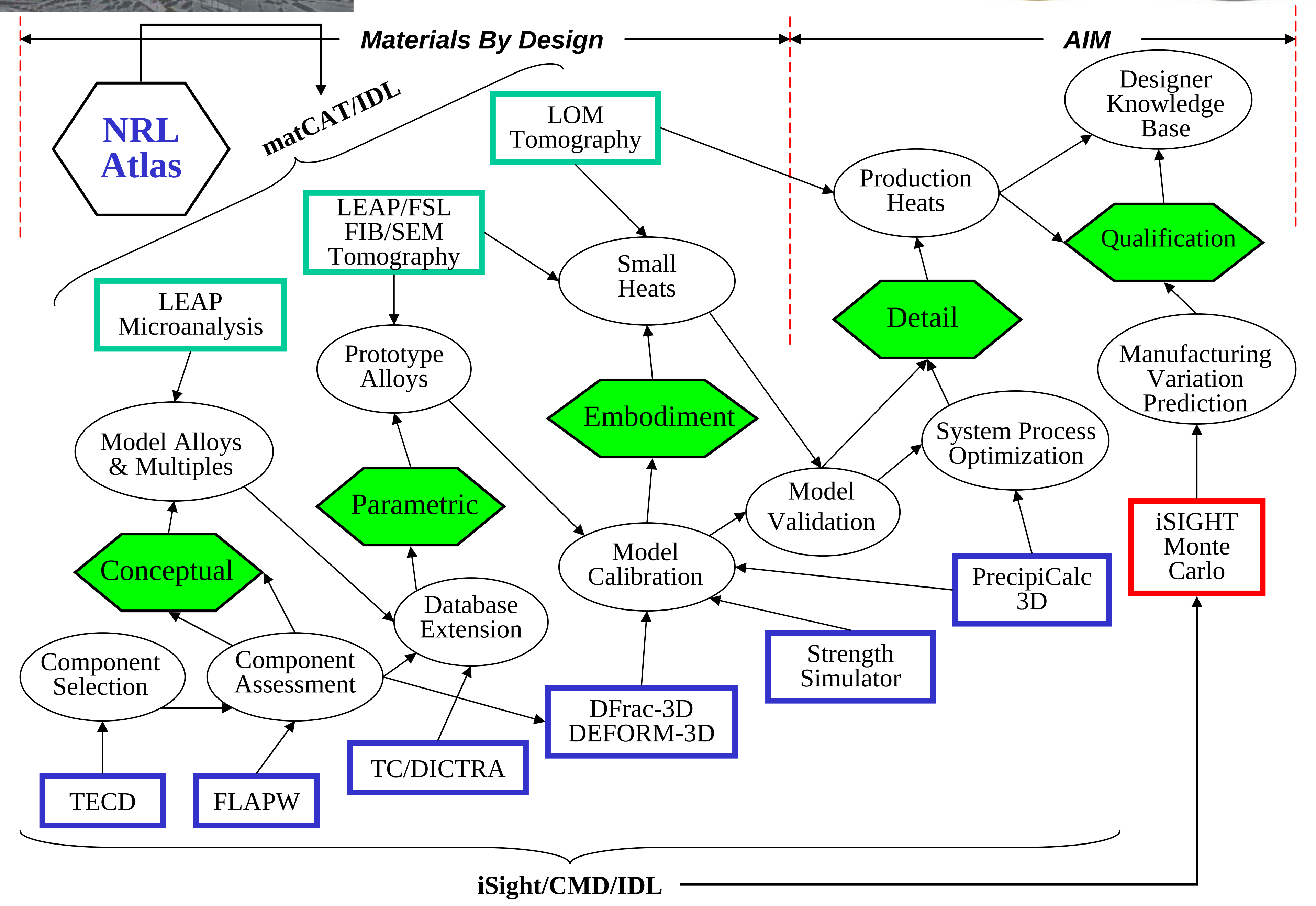
Overall Strategy for 3D Fatigue Modeling



Statistical estimates of cycles to crack formation with microstructure and spatial location

D.L. McDowell, Georgia Tech

Design Integration



The New Metallurgy
- Shifting the Core

Descriptive Science	→	Predictive Science
Exploration for Discovery	→	Pioneering by Design
Empirical Measurement	→	Validated Simulation
Deterministic Science	→	Probabilistic Science
Reductionist Analysis	→	Systems Synthesis
Knowledge Generation	→	Value Creation

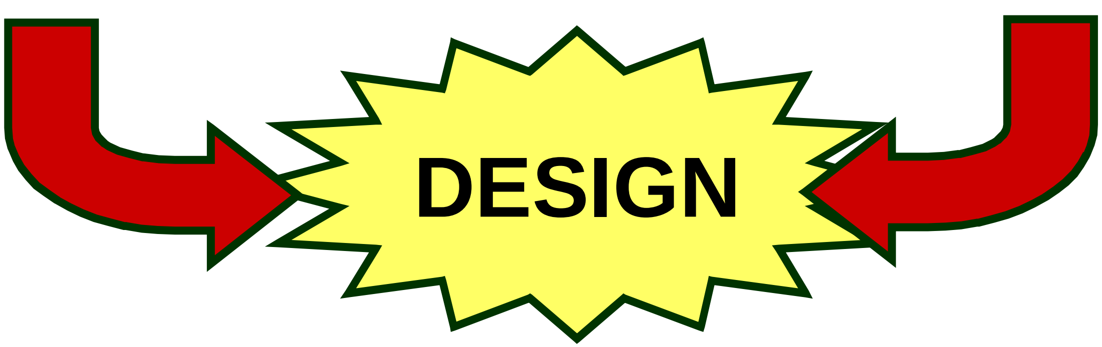
Our Vision: What an Engineer Should Be

Technical specialist

- Gets the job done!
- Can understand and analyze the physical and mathematical underpinnings of his/her field
- Works effectively with both the abstract and the physical
- Works problems through to a complete and realistic solution

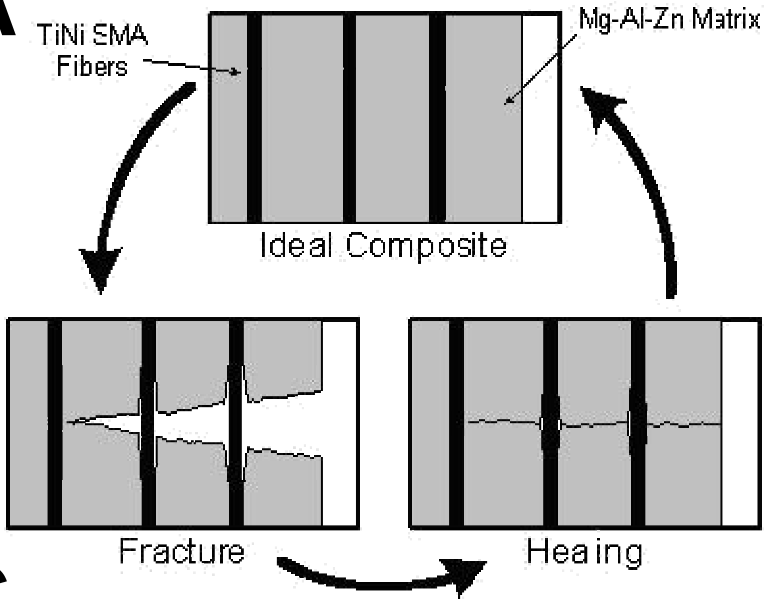
Creator of value

- Identifies and solves real problems within a social and economic context
- Works well in cross-disciplinary teams
- Adaptive learner
- Communicates effectively
- Responsible decision-maker

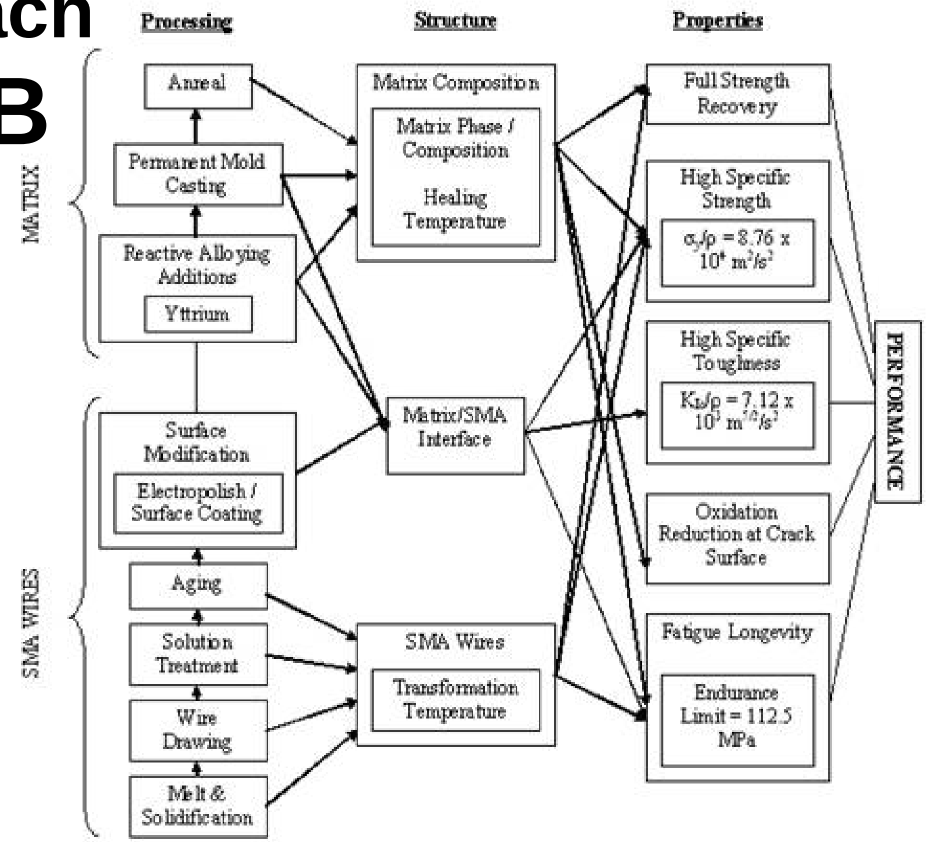


Systems Design Approach

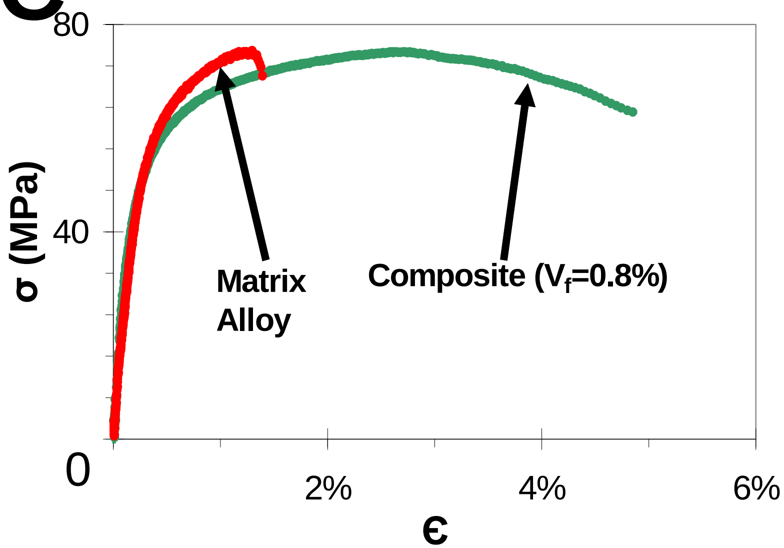
A



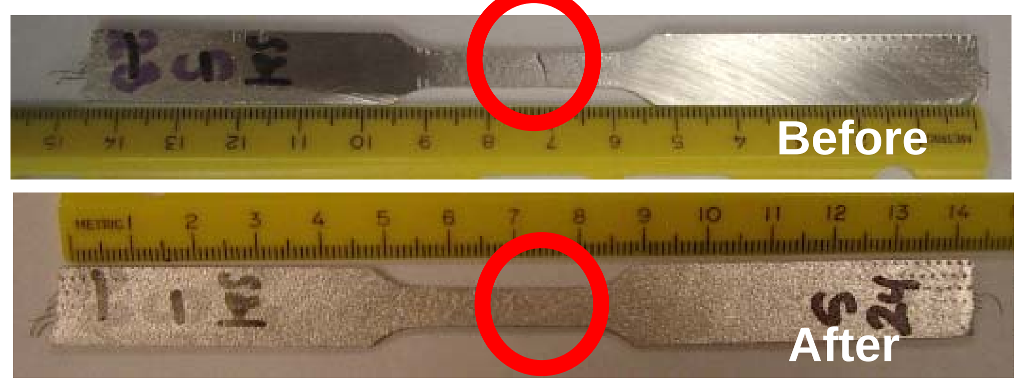
B



C



D

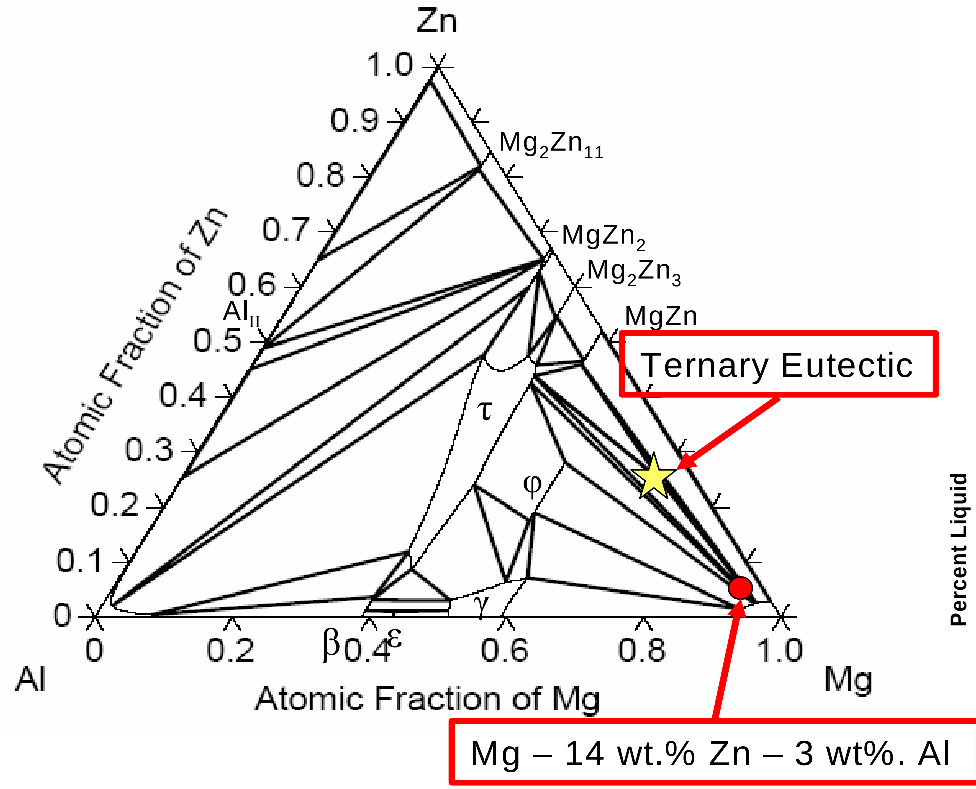


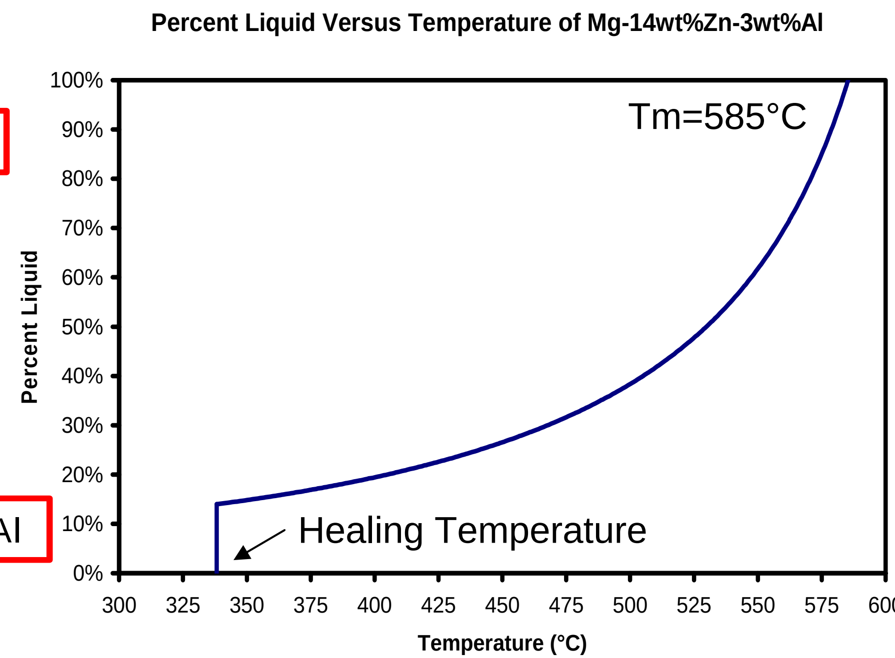
Successful Prototype. Sample demonstrates 98% strength recovery.

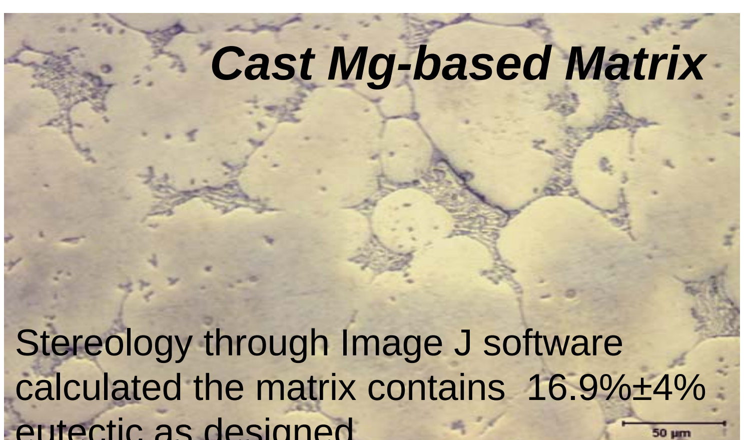
Computational Thermodynamic Design

Isothermal Section of Mg-Zn-Al Ternary System

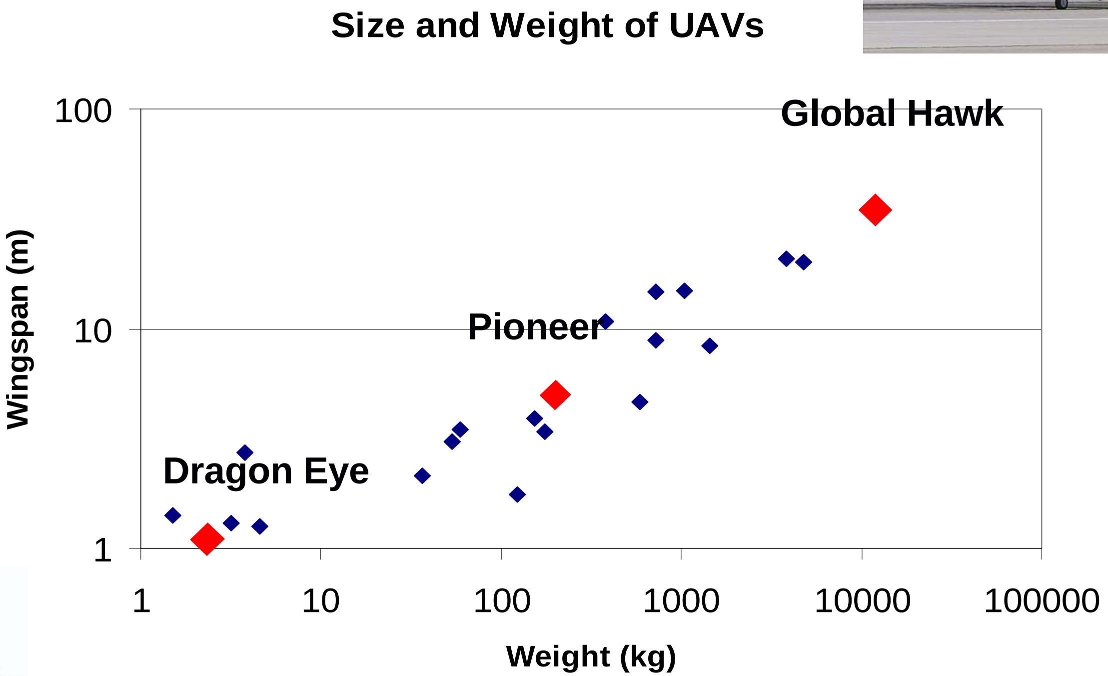
338°C







Unmanned Aerial Vehicles (UAVs)



- Survey of existing UAVs