COMPUTATIONAL MATERIALS DESIGN FOR ACCELERATED IMPLEMENTATION

G. B. Olson
Northwestern University / QuesTek Innovations LLC
Evanston IL

DOE SC-NE Workshop on Advanced Computational Mat. Sci.

March 31, 2004

MTL/SRG

A) Cybersteel 2020: Ultratough Plate Steels (ONR; CAT)
B) HT Carburizing Steels (DOE-OIT; GM, P&W)
C) Superalloys (AF-MEANS, DARPA-AIM; RMCI)
D) Bulk Metallic Glasses (DARPA-SAM)

GOVERNMENT

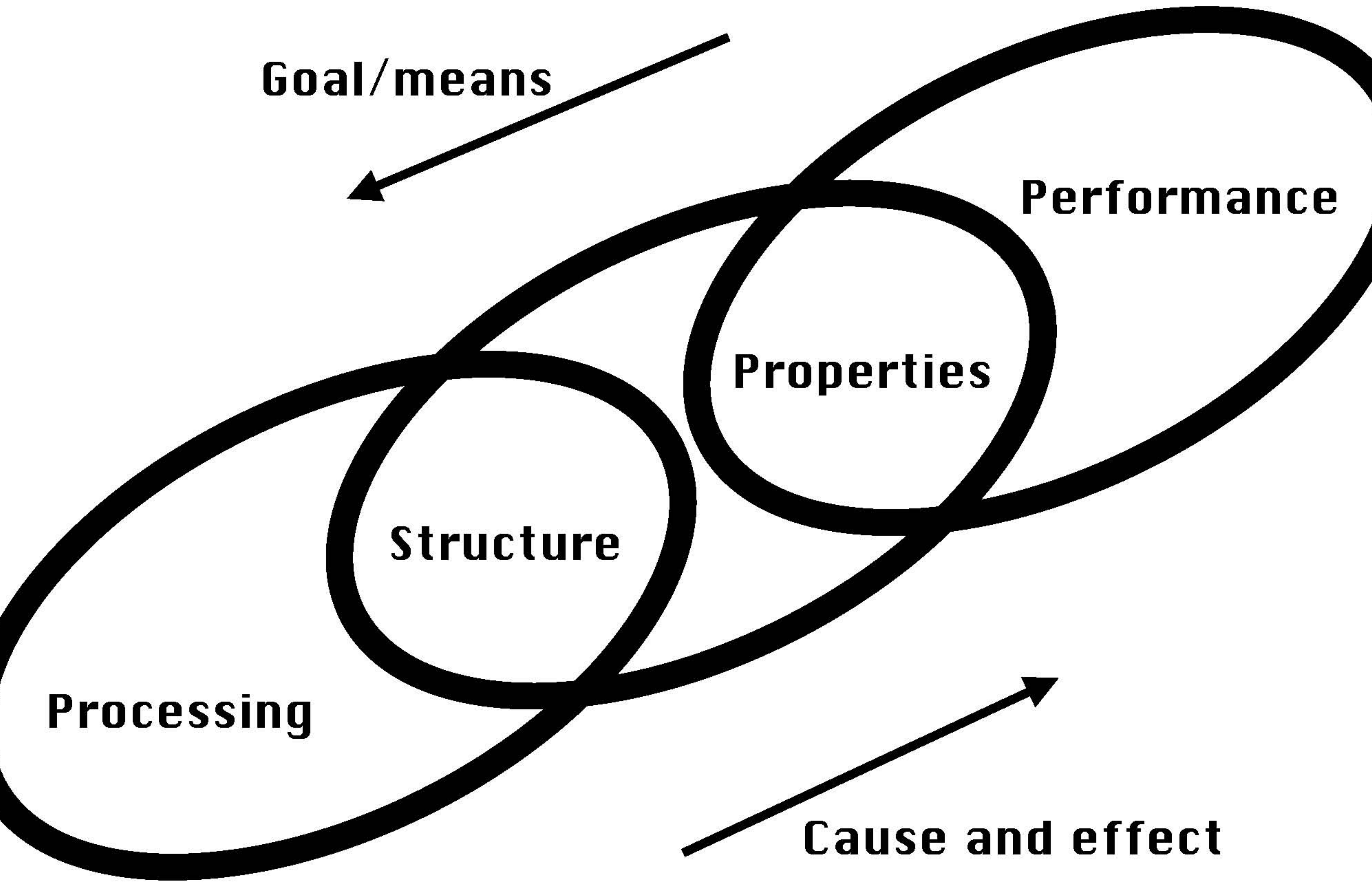
Organization	Projects	Members
NAWC/AD	A	Lee
ARL/WMD	B	Montgomery
AFRL	C,D	Woodward, Miracle

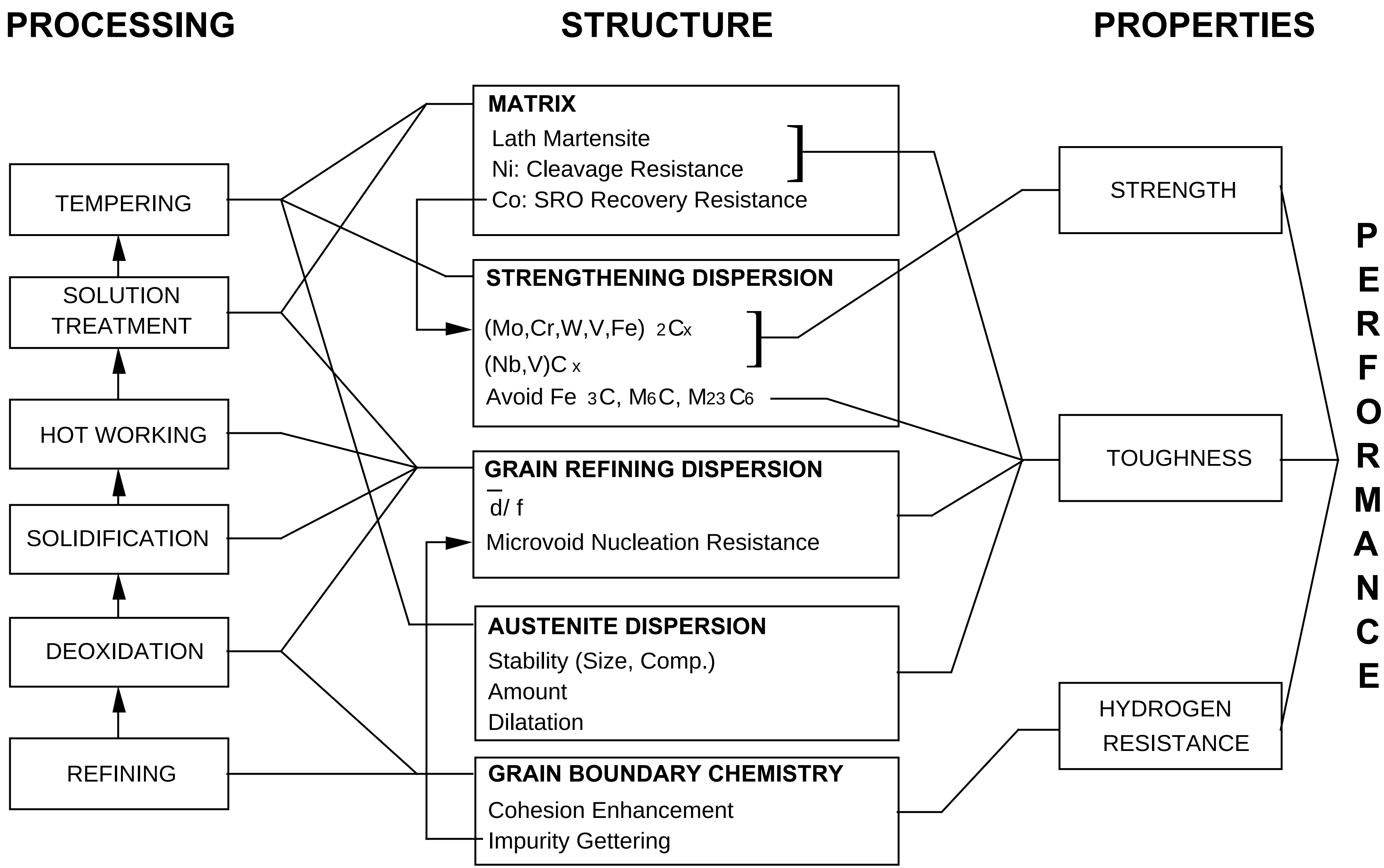
UNIVERSITY

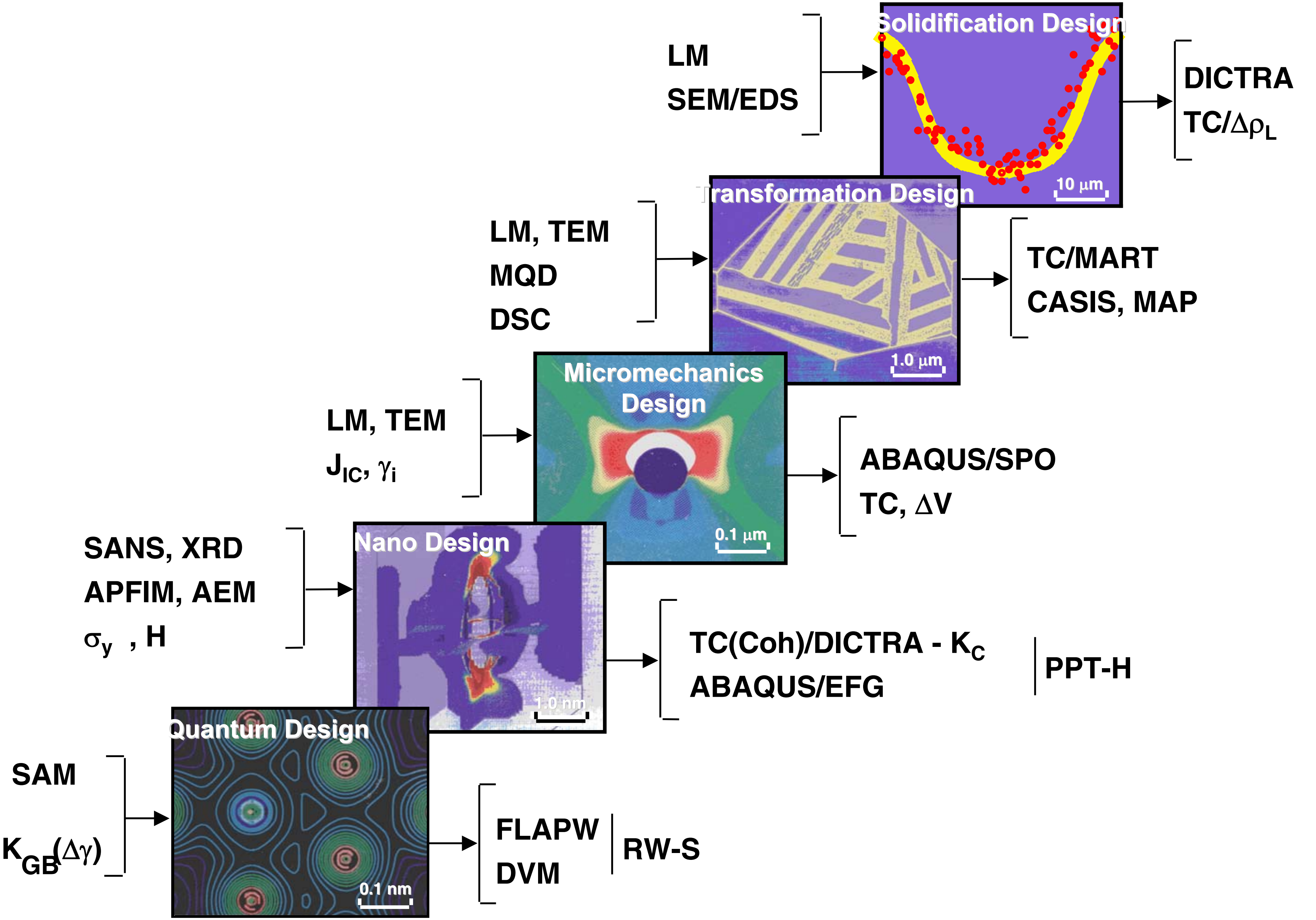
Organization	Projects	Members
NORTHWESTERN	A,B,C,D	Olson, Ankenman, Asta, Brinson, Dunand, Fine, Freeman, Ghosh, Isheim, Liu, Moran, Voorhees; High Resolution Microanalysis
WPI/CHTE	B	Apelian
PURDUE-CALUMET	B	Abramowitz
DREXEL	C	Doherty
KTH (Stockholm)	C	Agren, Sundman
LEHIGH	C	Harlow
OHIO STATE	C	Fraser, Mills
CSM	C	Eberhart
WISCONSIN-MAD	C,D	Perepezko
MIT	D	Argon, Parks
IIT	D	Nash
VIRGINIA	D	Poon, Shiflet

INDUSTRY

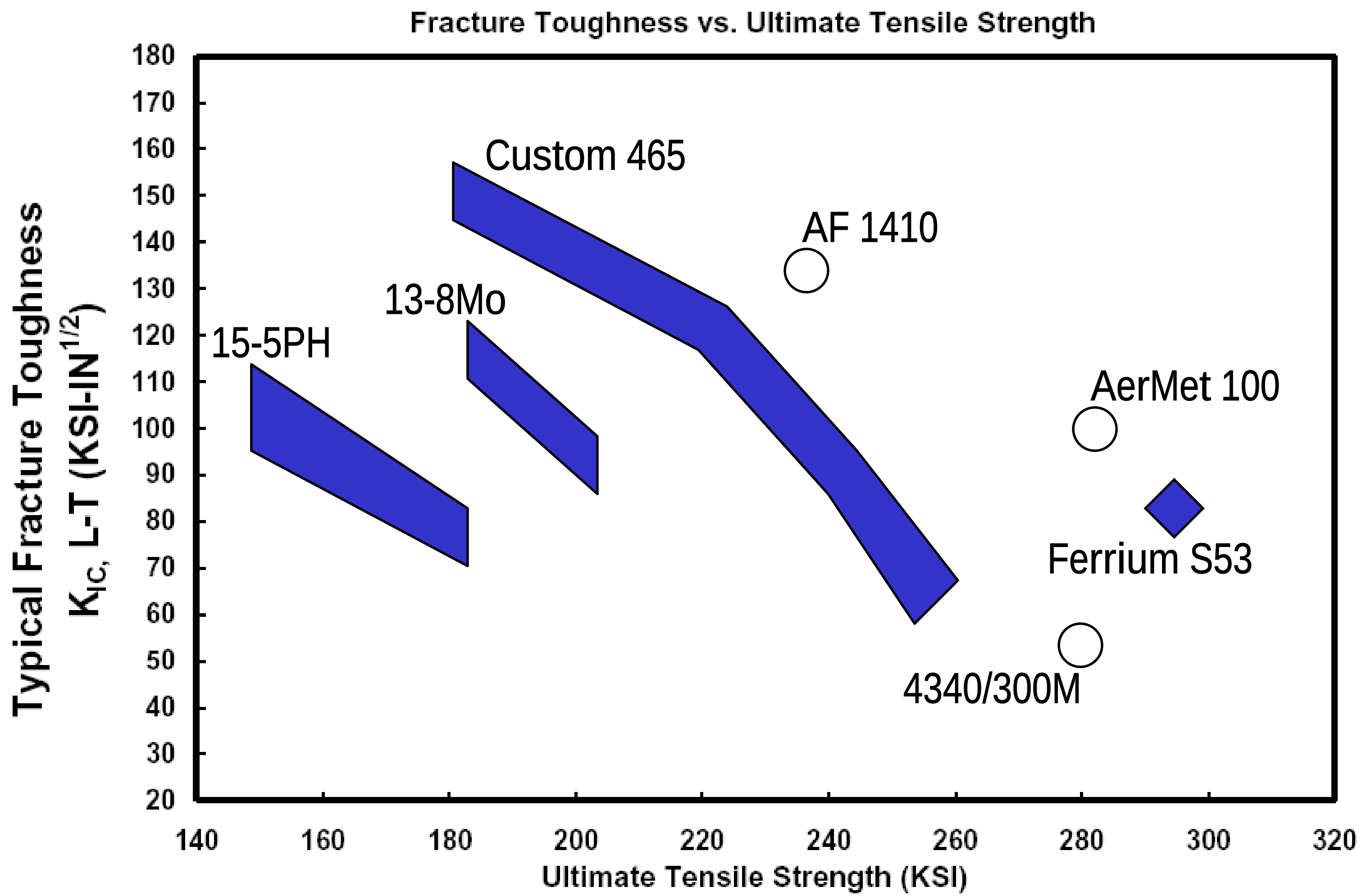
Organization	Projects	Members
QUESTEK	A,B,C,D	Kuehmann, Huang, Jou, Qiu, Rathbun, Scharer, Tang, Tufts, Wright
CATERPILLAR	A,B	Chen, Hsieh, Johnson, Yang
ALLVAC STEEL	A,B	Lippard, Stevenson
INLAND STEEL	A	Bhattacharya
GM	B	Mishra, Sachdev
PRATT & WHITNEY	B,C,D	Fowler, Schirra
REFERENCE METALS	C	Carneiro
HOWMET	D	Wolter, Wright
BOEING	D	Bowden

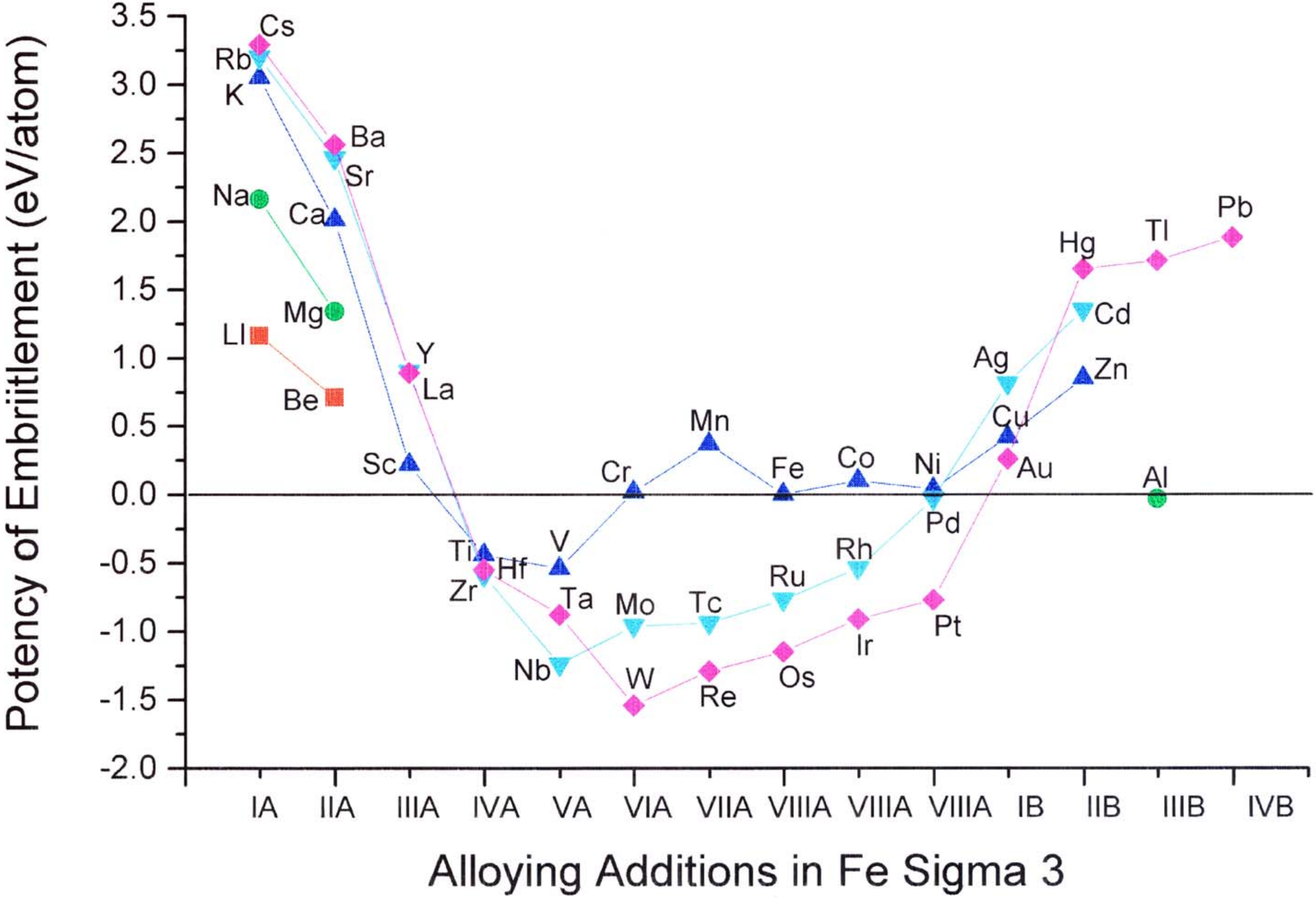

Goal/means
Performance
Properties
Structure
Processing
Cause and effect


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) $_2C_x$
(Nb,V)C_x
Avoid Fe_3C, M_6C, $M_{23}C_6$
GRAIN REFINING DISPERSION
$\bar{d}/f$
Microvoid Nucleation Resistance
AUSTENITE DISPERSION
Stability (Size, Comp.)
Amount
Dilatation
GRAIN BOUNDARY CHEMISTRY
Cohesion Enhancement
Impurity Gettering
STRENGTH
TOUGHNESS
HYDROGEN RESISTANCE
PERFORMANCE

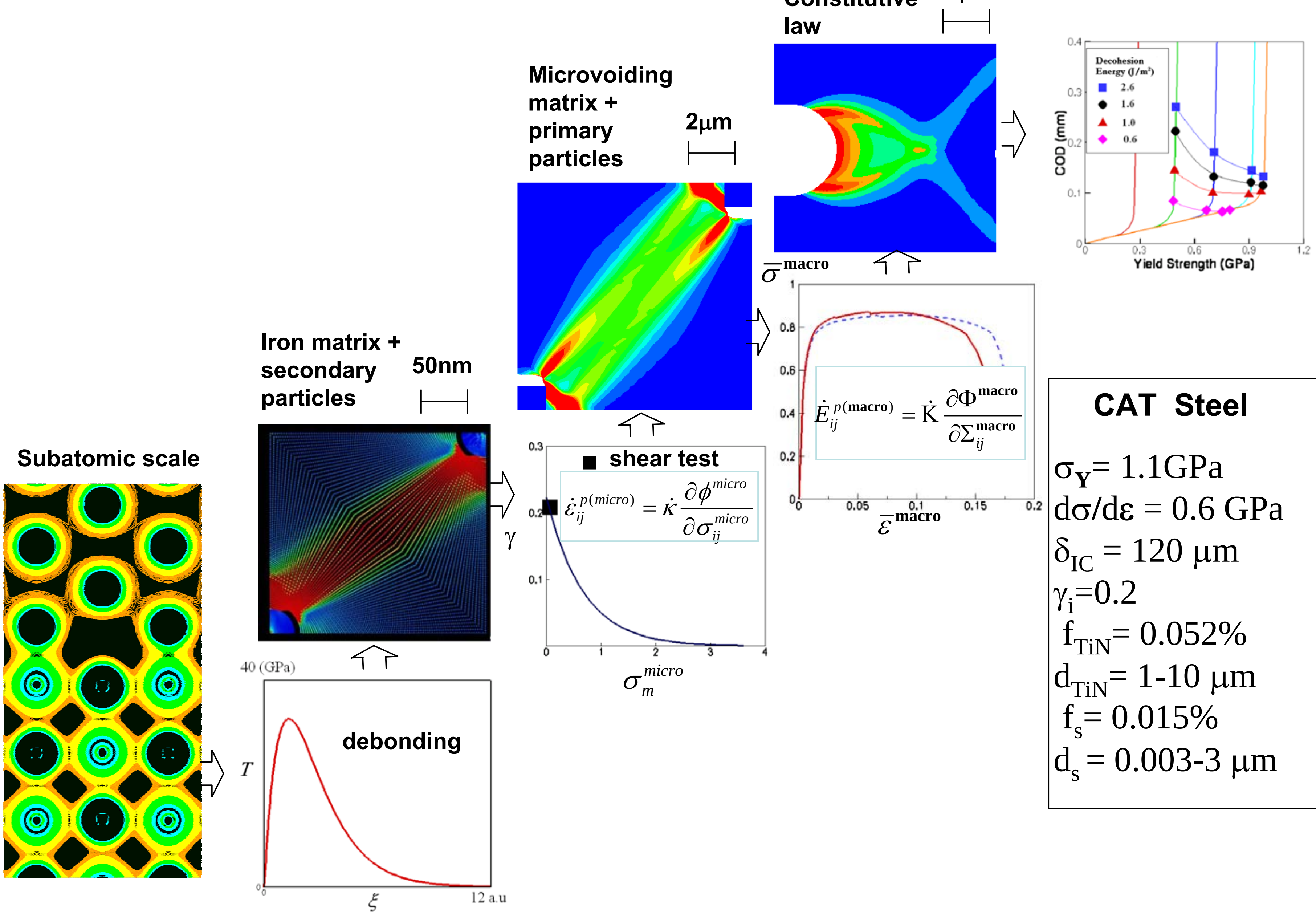

LM
SEM/EDS
Solidification Design
10 μm
DICTRA
TC/ΔρL
LM, TEM
MQD
DSC
Transformation Design
1.0 μm
TC/MART
CASIS, MAP
LM, TEM
JIC, γi
Micromechanics Design
0.1 μm
ABAQUS/SPO
TC, ΔV
SANS, XRD
APFIM, AEM
σy , H
Nano Design
1.0 nm
TC(Coh)/DICTRA - KC
ABAQUS/EFG
PPT-H
SAM
KGB(Δγ)
Quantum Design
0.1 nm
FLAPW
DVM
RW-S

S53 Nanostructured UHS Stainless Results




Potency of Embrittlement (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
W
Cr
Mo
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

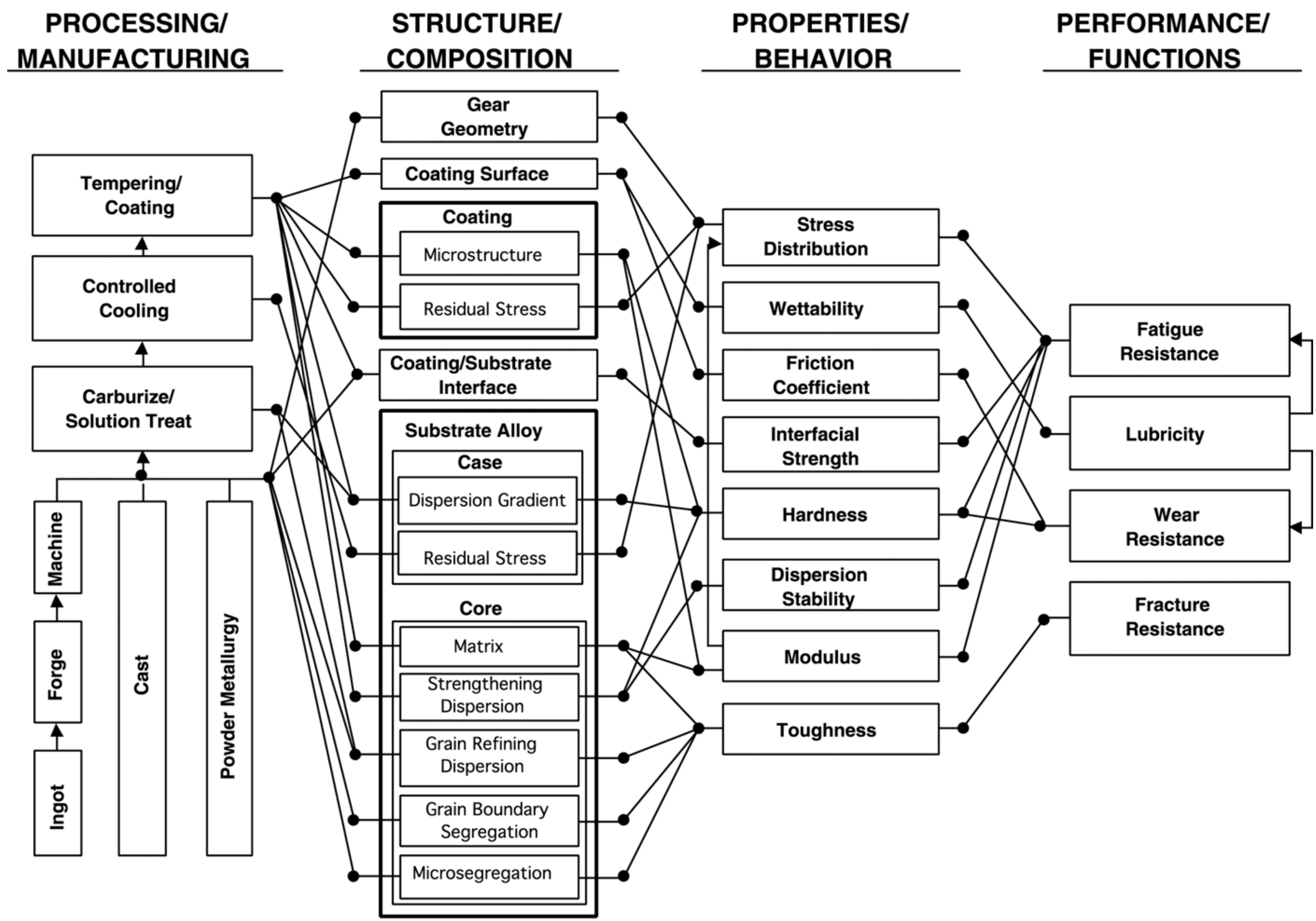
Multiscale Ductile Fracture Simulator



CAT Steel

σ_Y = 1.1GPa
$d\sigma/d\varepsilon$ = 0.6 GPa
δ_{IC} = 120 μm
γ_i=0.2
f_{TiN}= 0.052%
d_{TiN}= 1-10 μm
f_s= 0.015%
d_s = 0.003-3 μm

HIGH POWER-DENSITY GEARS



Current Applications

Gears: NASCAR

-Successfully completed race with narrow gear design

-Moving forward with development

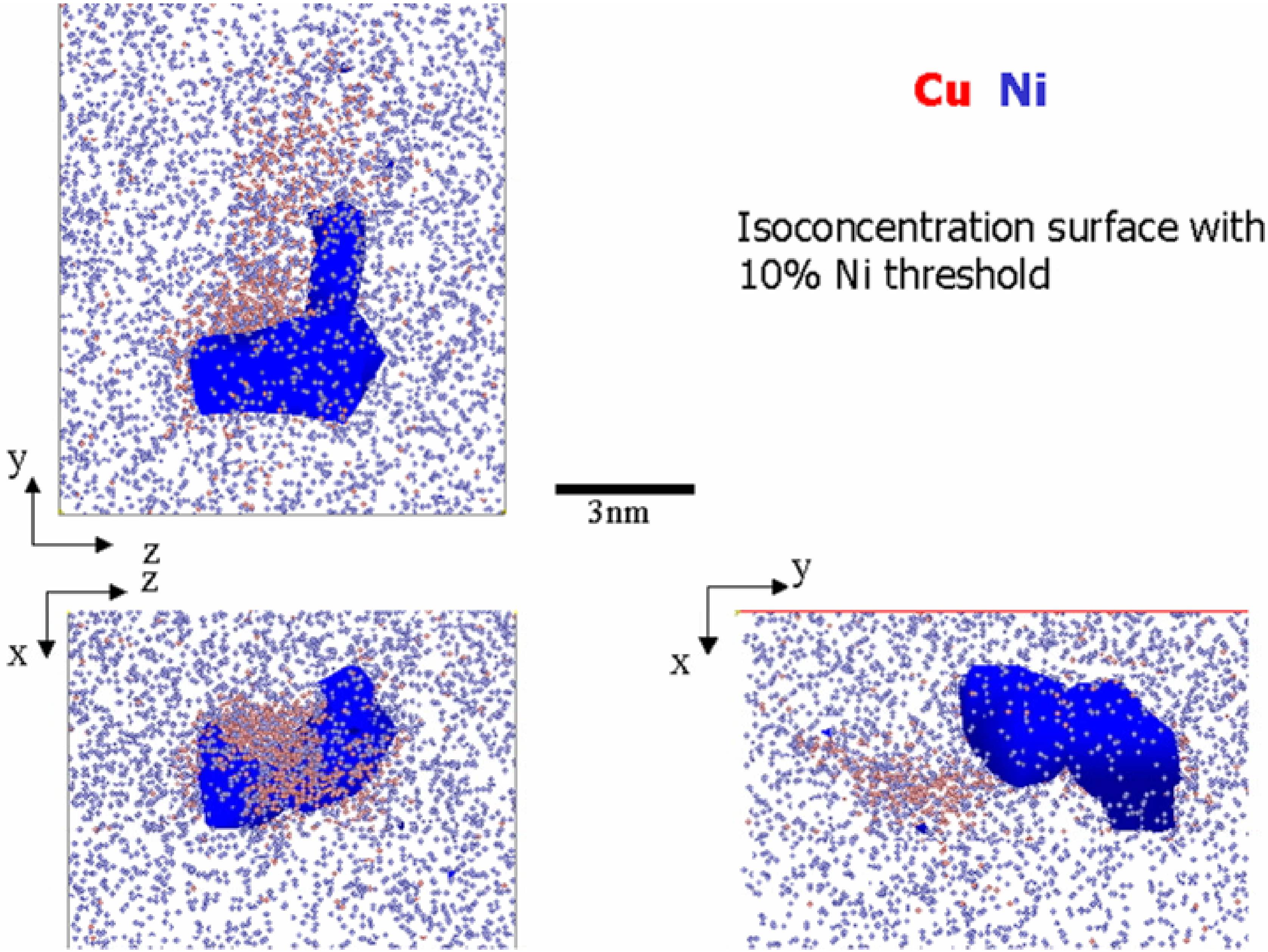
Ring & Pinion: SCORE

-Finished entire race with new design

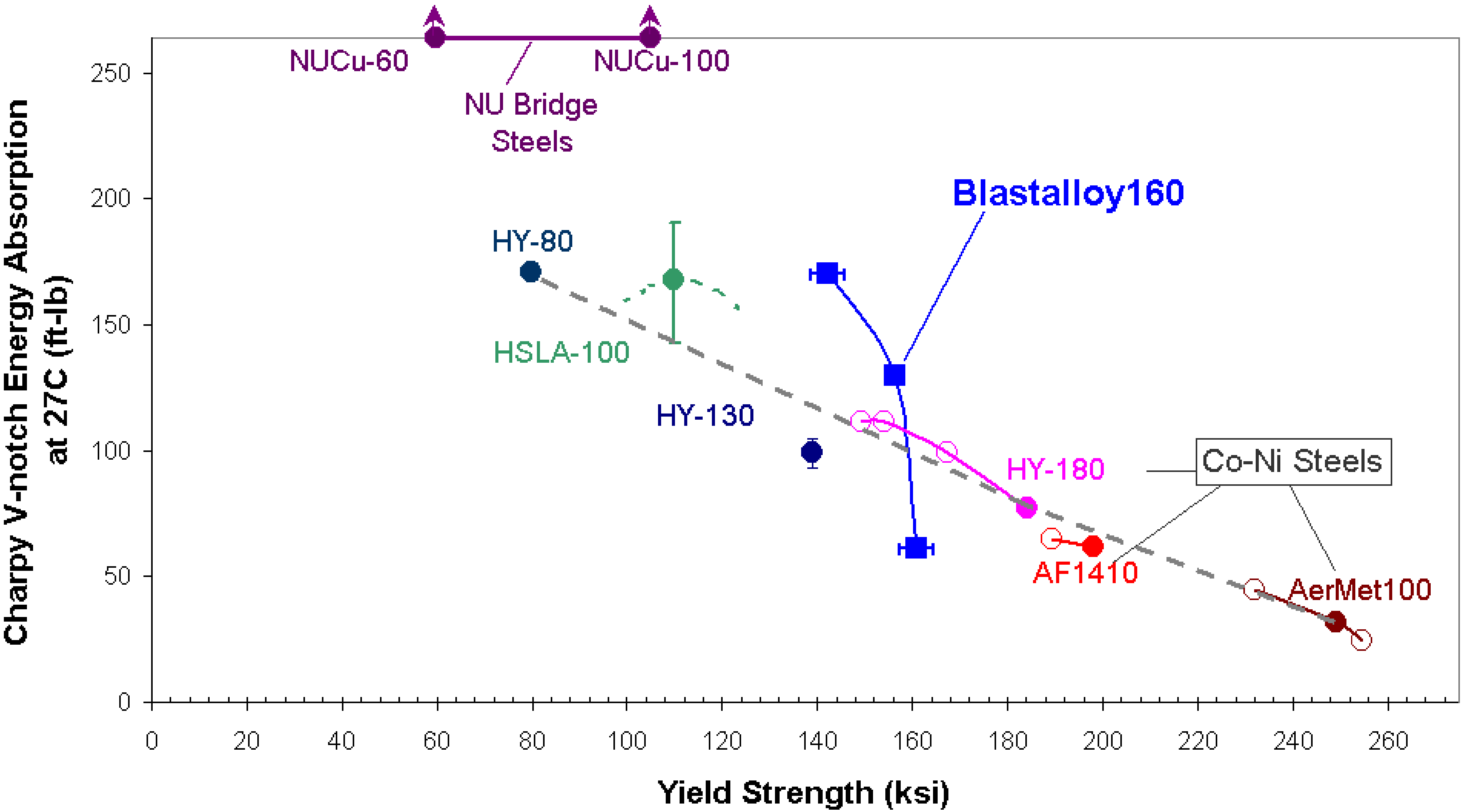
-Production sets being made

Dog Rings and Camshafts: Currently in testing

Heterogeneous Precipitation of Austenite on Copper Particles



Toughness - Strength Combination



ARCHITECTURE DESIGN

Integration Infrastructure

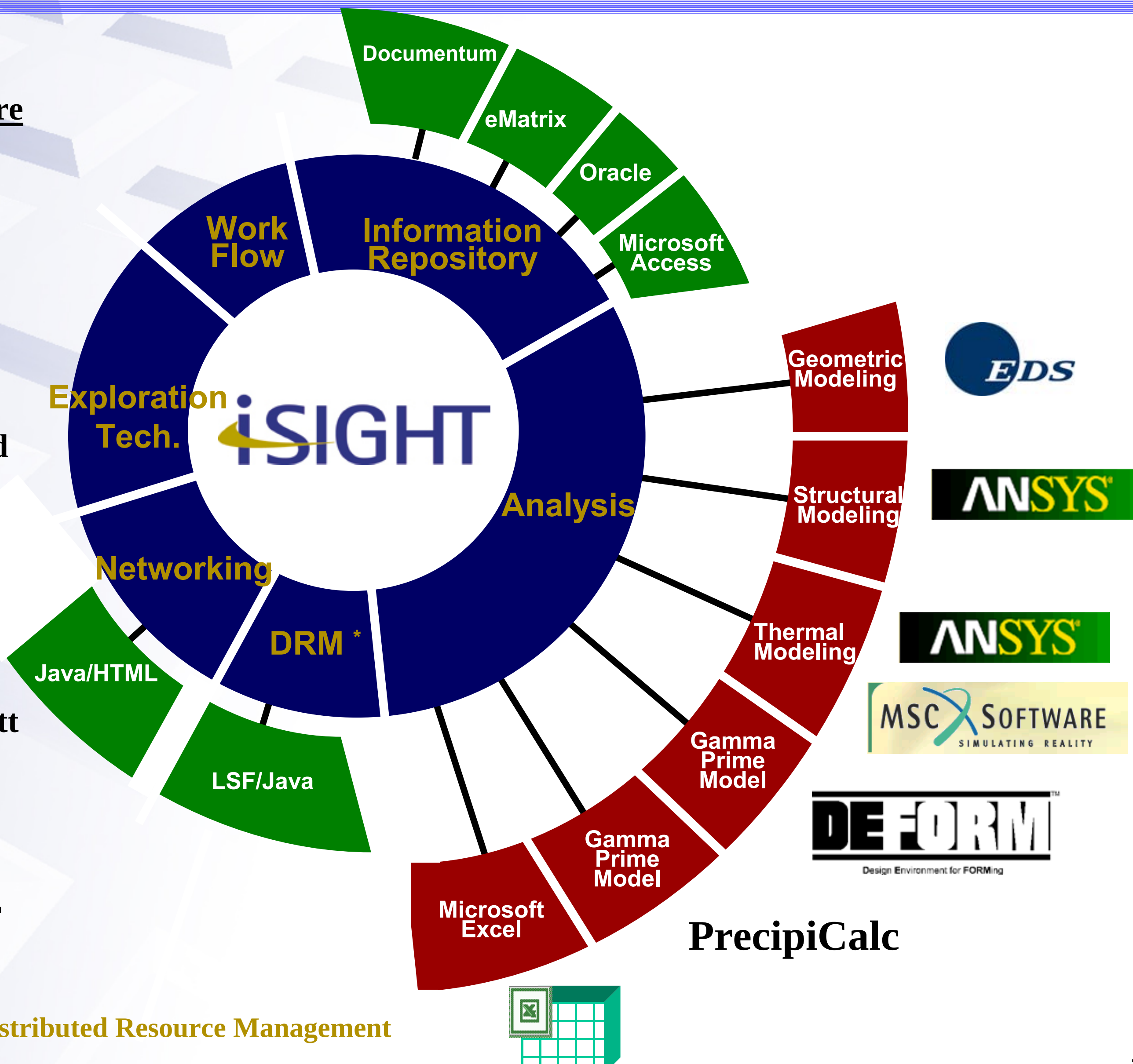
iSIGHT framework provided by Engineous Software

Core Utilities

3RD Party tools to extend iSIGHT's integration capabilities

Analysis Components

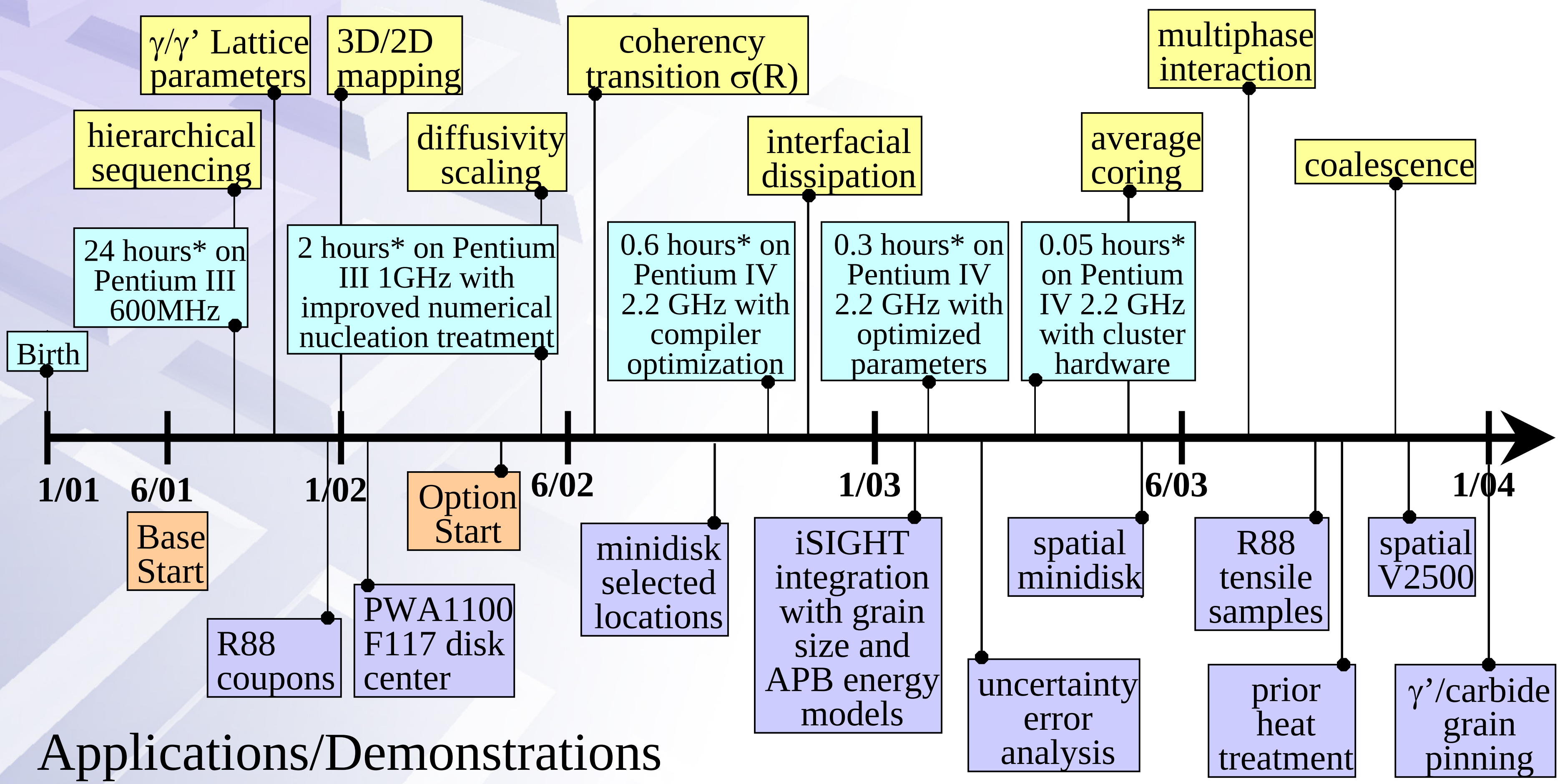
Models provided by Pratt & Whitney, General Electric, Questek, and others. Integrated by Engineous into the DKB architecture via iSIGHT



* Distributed Resource Management

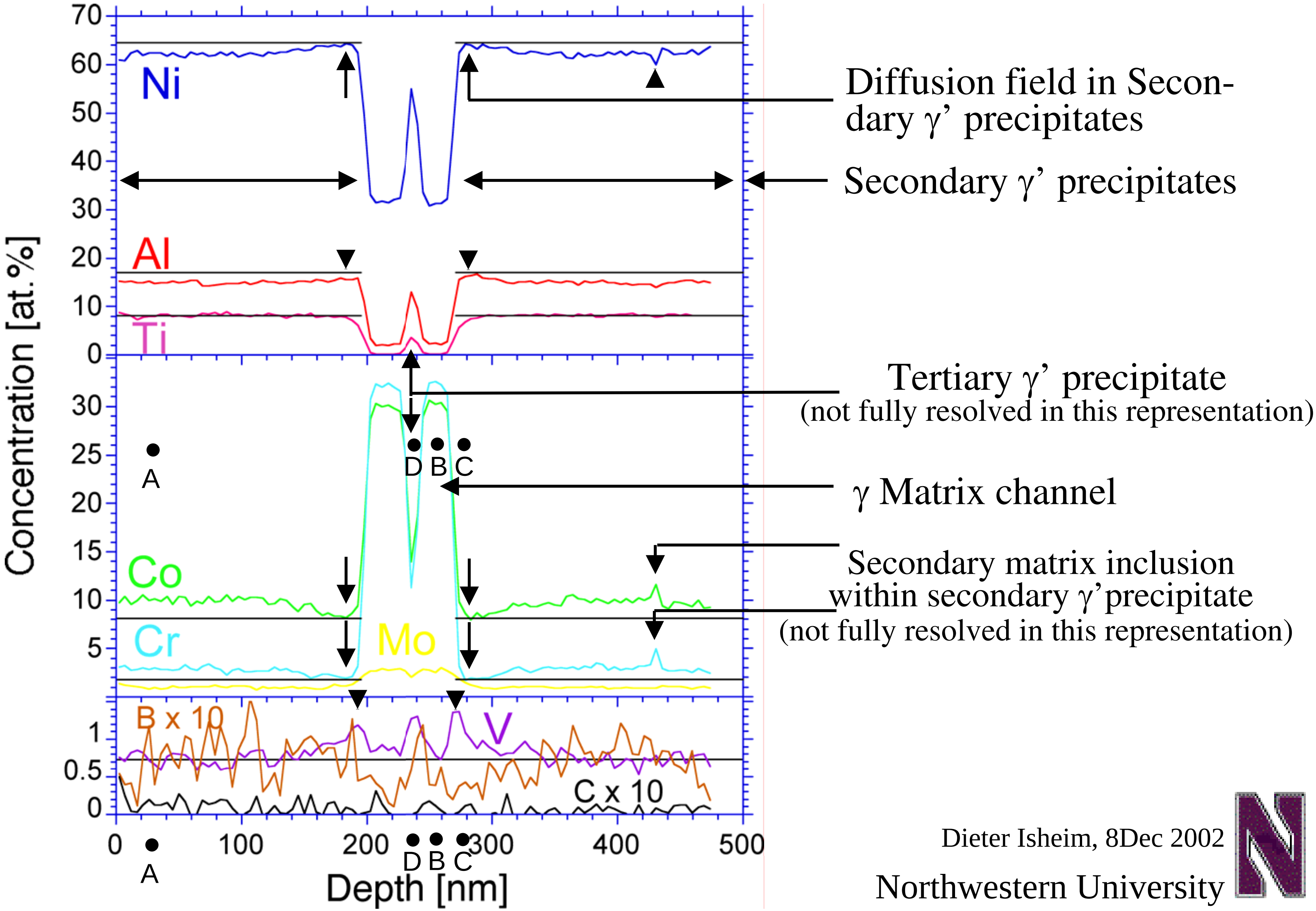
PrecipiCalc™ Timeline

Software/Hardware Improvement



* single IN100 PWA1100 simulation

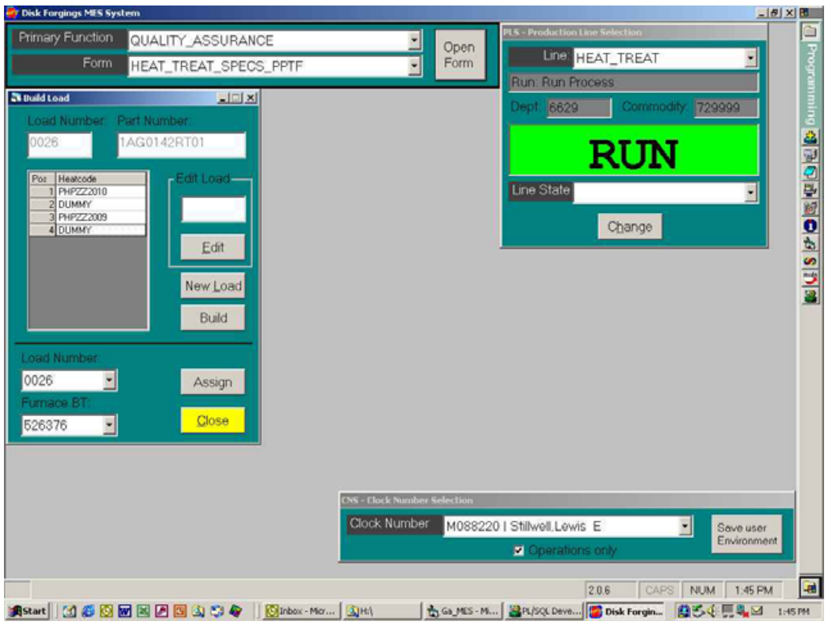
Composition Profile (at.%) across Matrix Channel in between Secondary Precipitates w. Tertiary Precipitate in IN100 - Center 1st Disc

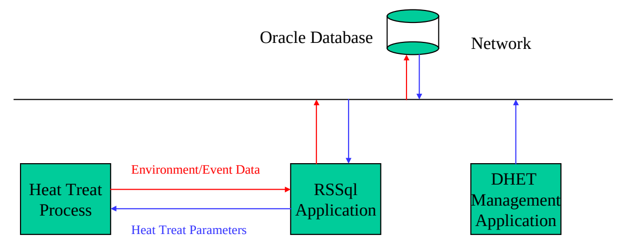


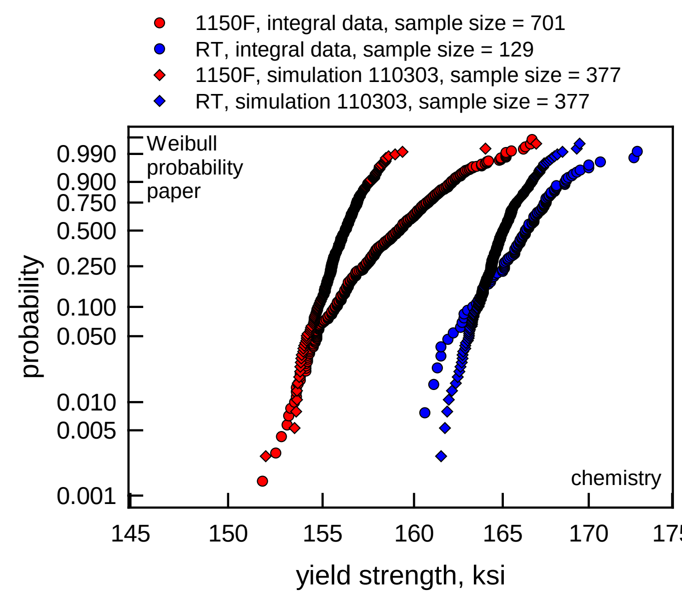
Dieter Isheim, 8Dec 2002
Northwestern University

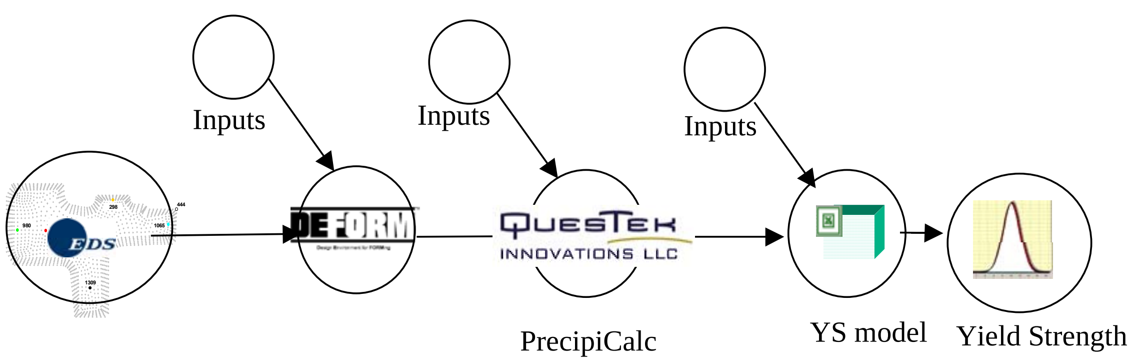
Impact of DARPA AIM Initiative

- Supply chain impact on material capability captured
  - ➢Enables versatile processing for smaller lot sizes

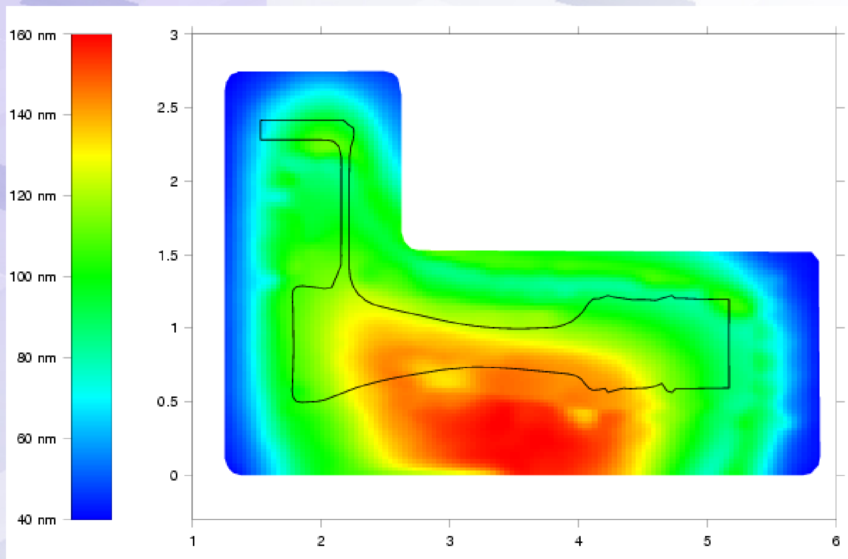


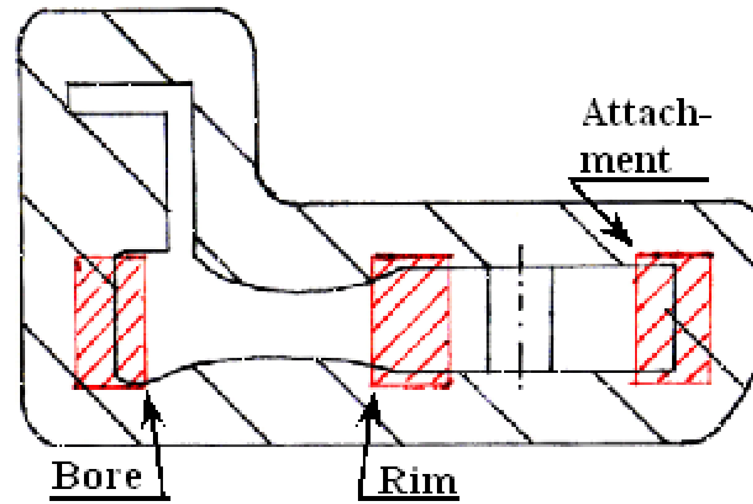






Minidisk Microstructure Prediction with *PrecipiCalc*

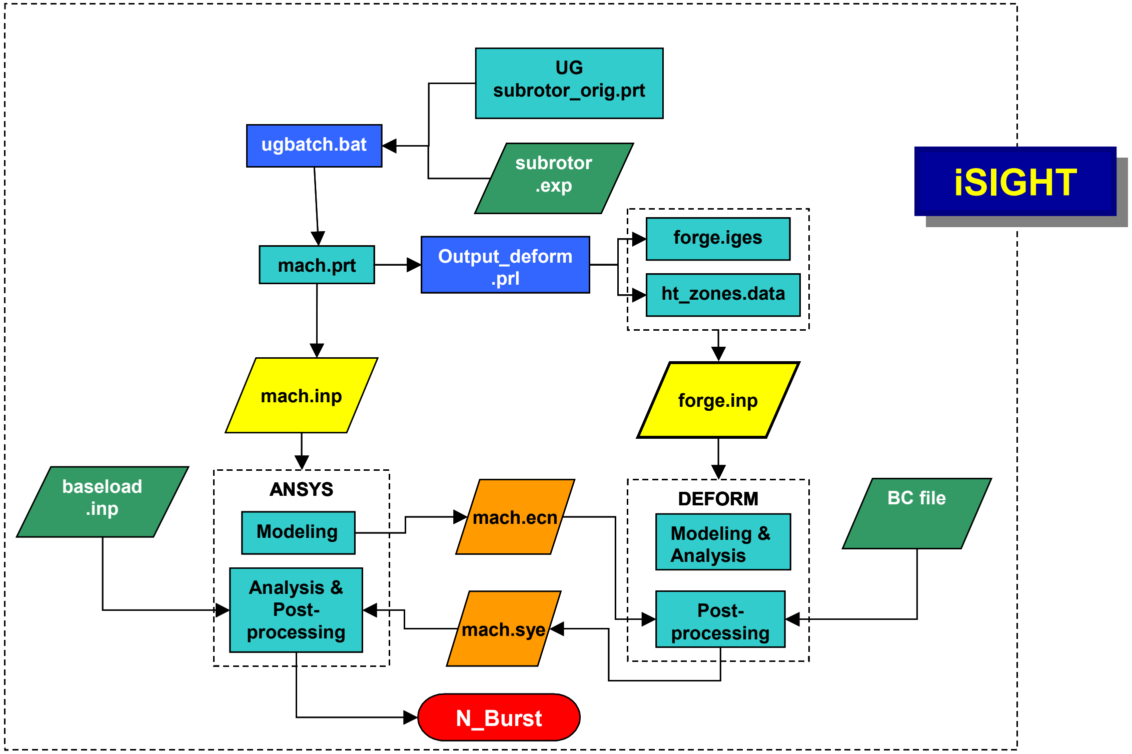


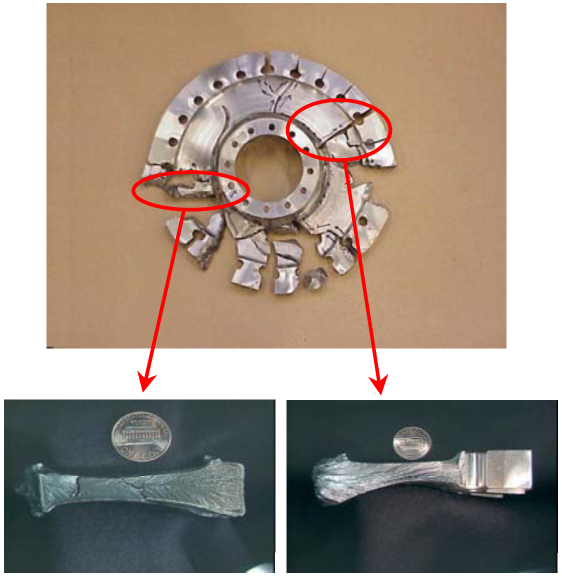


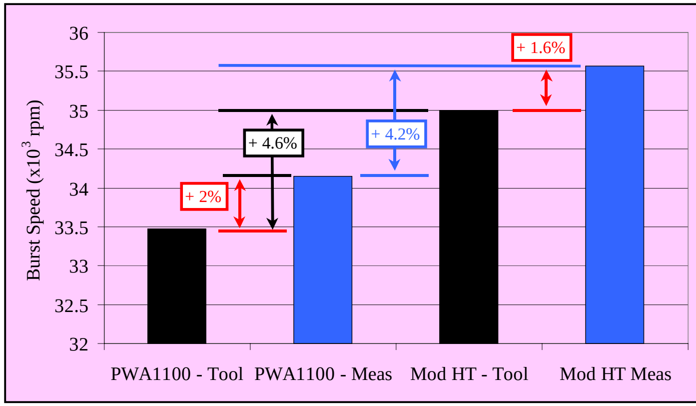
Minidisk Comparison		Bore		Rim		Attachment	
		Exp.	PpC	Exp.	PpC	Exp.	PpC
Primary γ’	Fraction (%)	24 25.2	22.6	23.5 25	23.5	23.1 25.7	23.3
	Size (μm)	1.28	1.29	1.23 1.27	1.32	1.18 1.2	1.31
Secondary γ’	Fraction (%)	32.4	35		34		34.6
	Size (nm)	109 129	107.9	132 157	120 135 146	103 114	84.2
Tertiary γ’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

Impact of DARPA AIM Initiative

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







S53: Example Variation Analysis

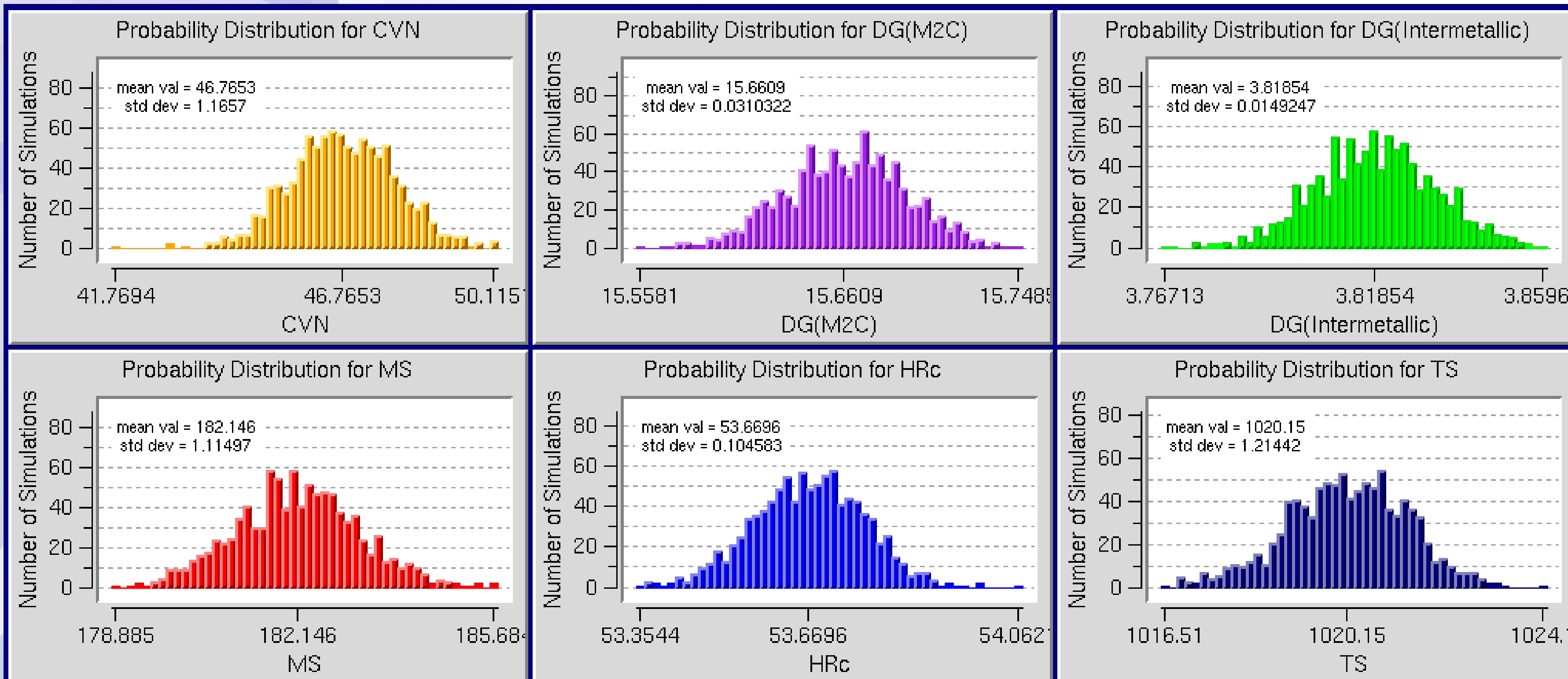
Compositional Variations (wt%, ±6σ):

C	± 0.01	**Cr**	± 0.2	**Mo**	± 0.1
W	± 0.1	**Co**	± 0.3	**Ni**	± 0.1
V	±0.02				

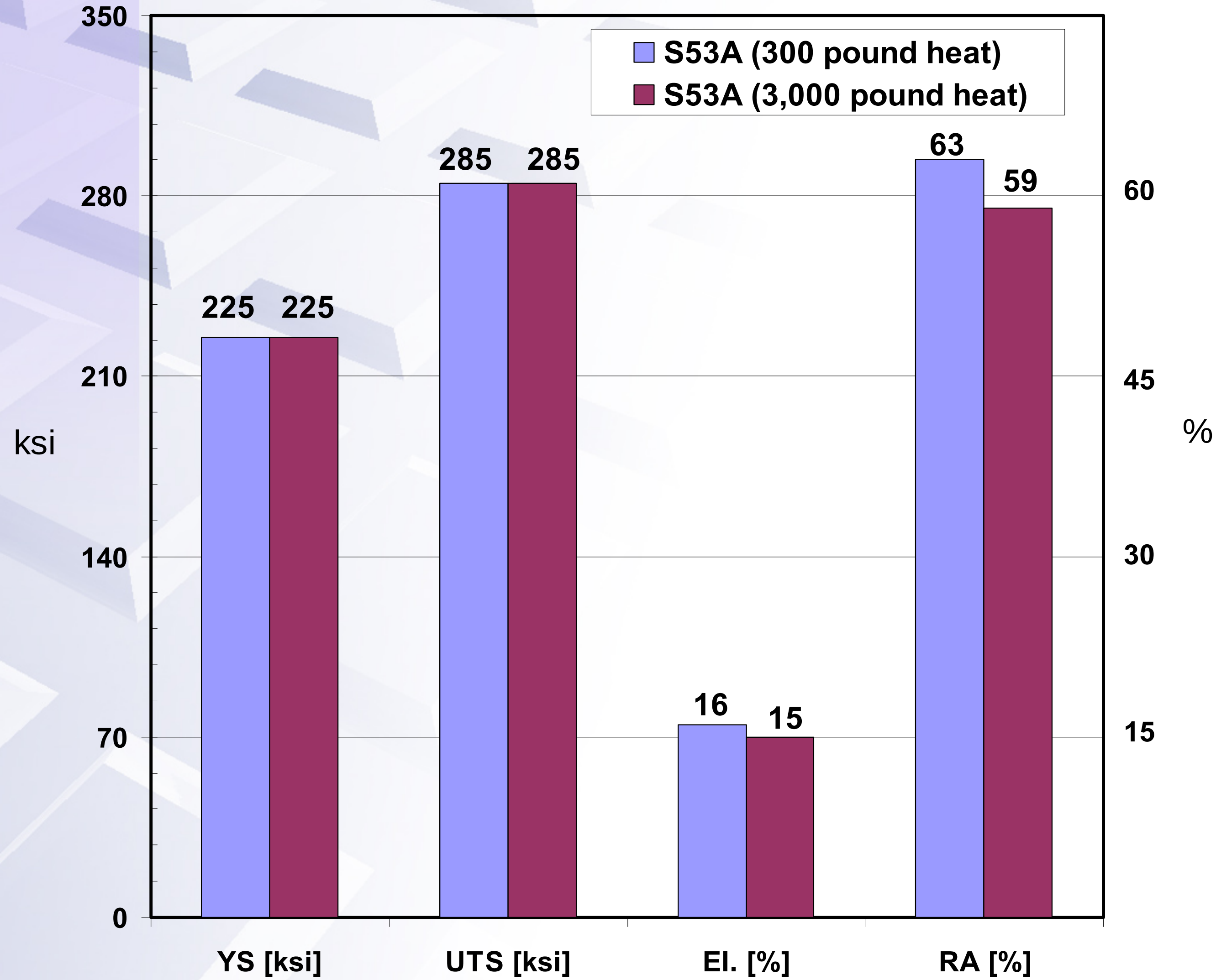
CMD/ iSIGHT

Variations of:
Structure — carbide solvus Ts**,** martensite Ms, precipitation control ΔG's
Property — hardness HRc, toughness CVN

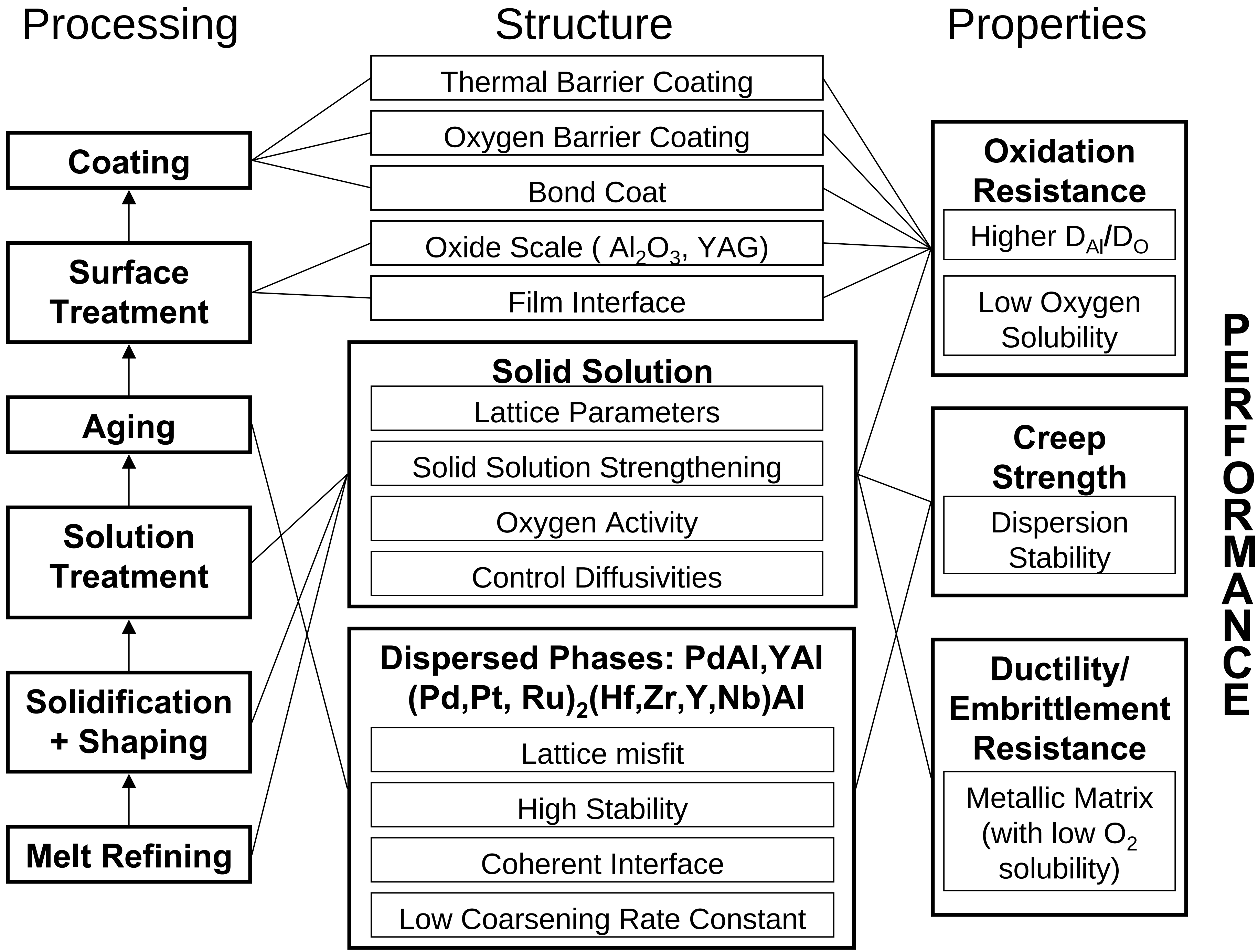
Results of 1000 runs (12 minutes on a Pentium IV 2.2GHz CPU)

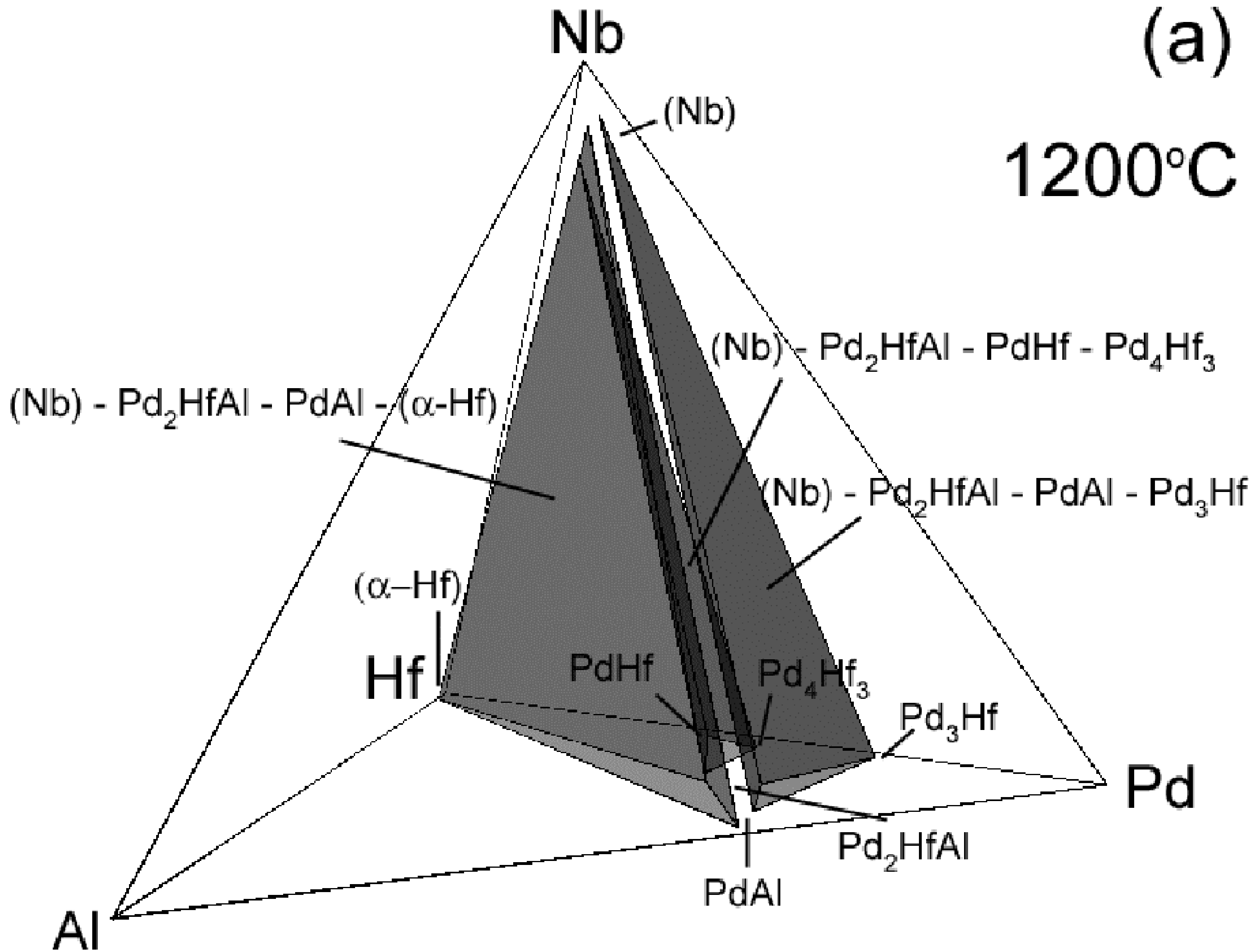


S53A Scale-up Properties

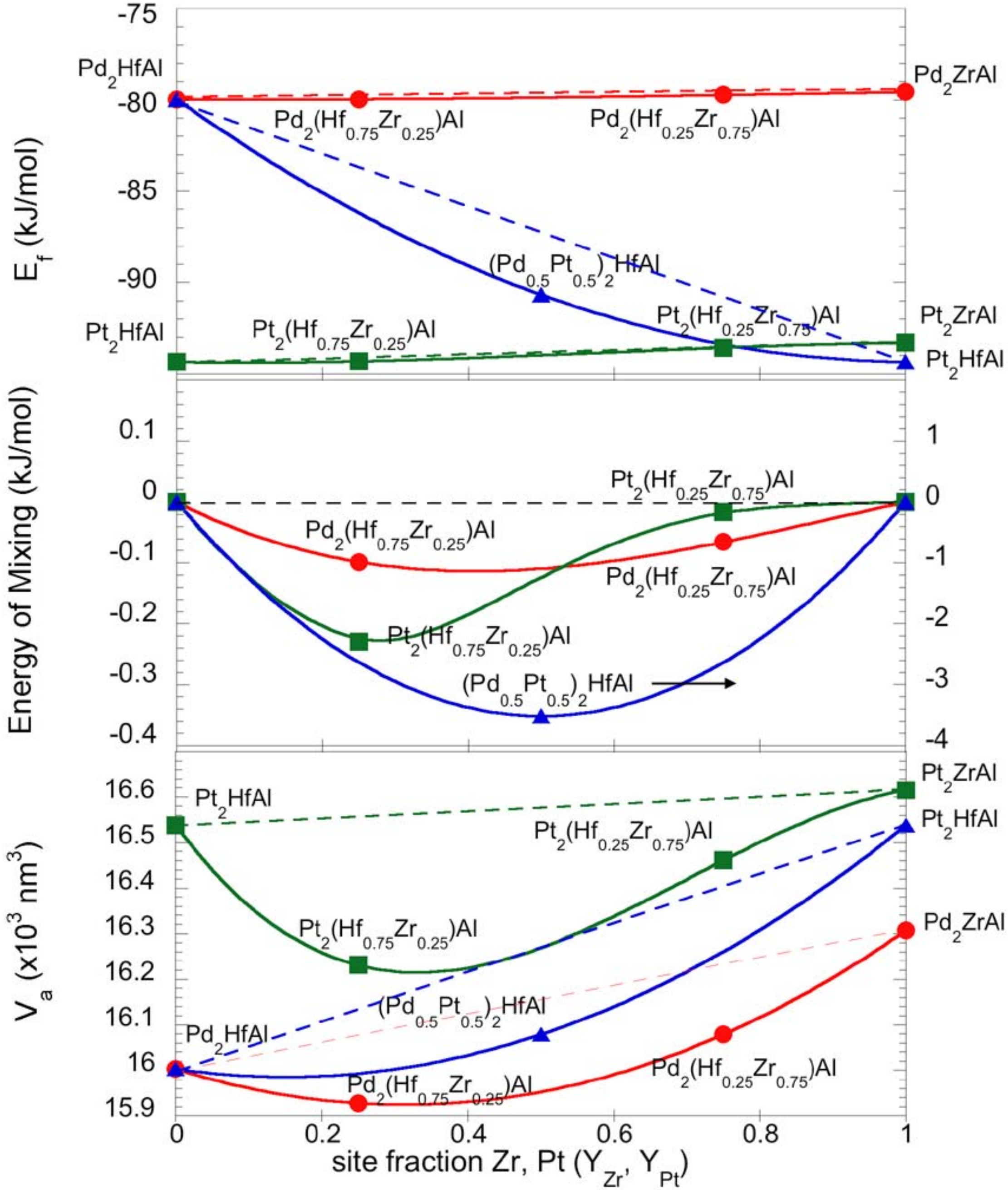


QuesTek INNOVATIONS LLC

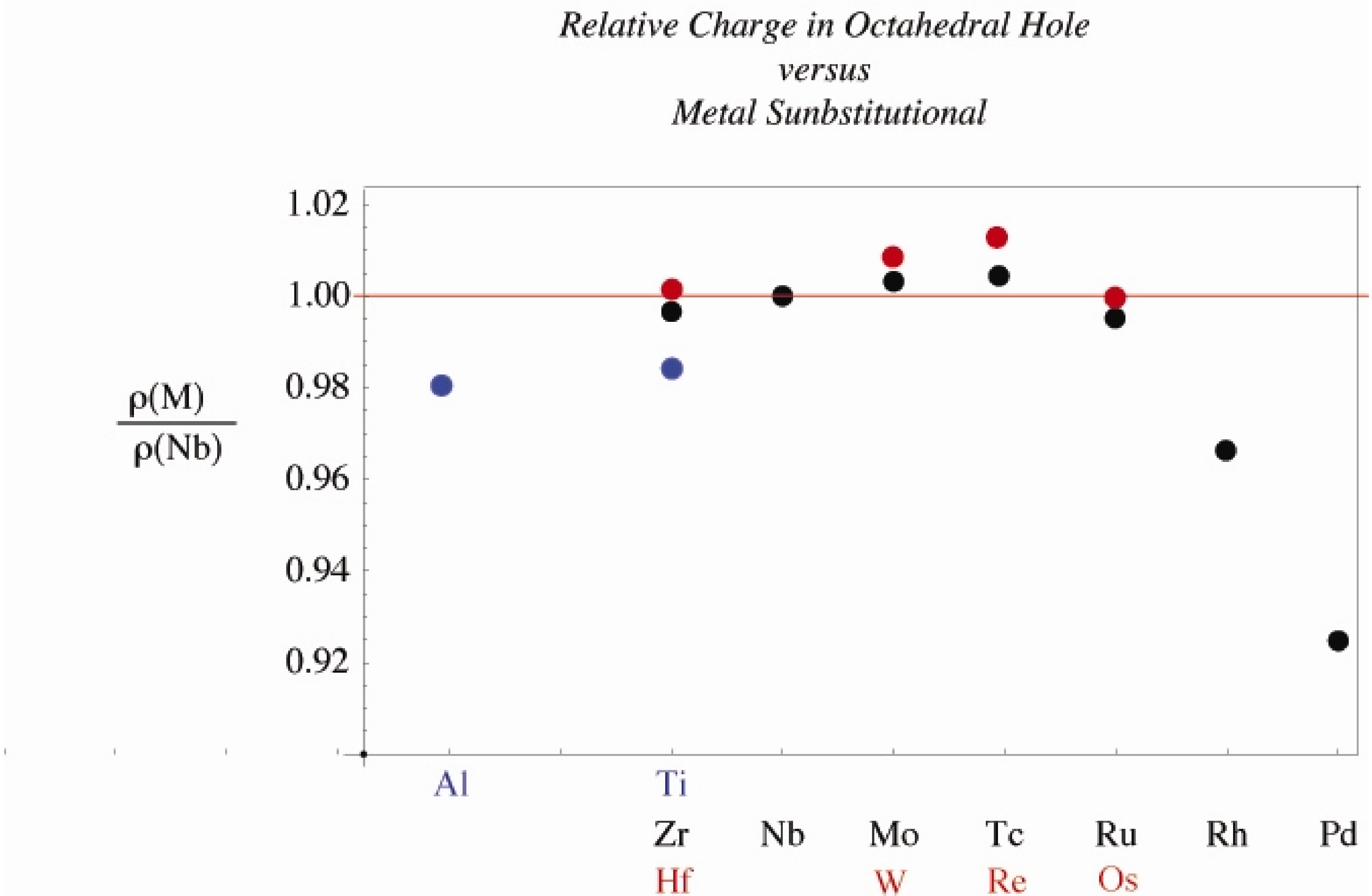

Processing
Structure
Properties
Coating
Surface Treatment
Aging
Solution Treatment
Solidification + Shaping
Melt Refining
Thermal Barrier Coating
Oxygen Barrier Coating
Bond Coat
Oxide Scale (Al_2O_3, YAG)
Film Interface
Solid Solution
Lattice Parameters
Solid Solution Strengthening
Oxygen Activity
Control Diffusivities
Dispersed Phases: PdAl,YAl
$(Pd,Pt, Ru)_2(Hf,Zr,Y,Nb)Al$
Lattice misfit
High Stability
Coherent Interface
Low Coarsening Rate Constant
Oxidation Resistance
Higher D_{Al}/D_O
Low Oxygen Solubility
Creep Strength
Dispersion Stability
Ductility/ Embrittlement Resistance
Metallic Matrix (with low O_2 solubility)
PERFORMANCE

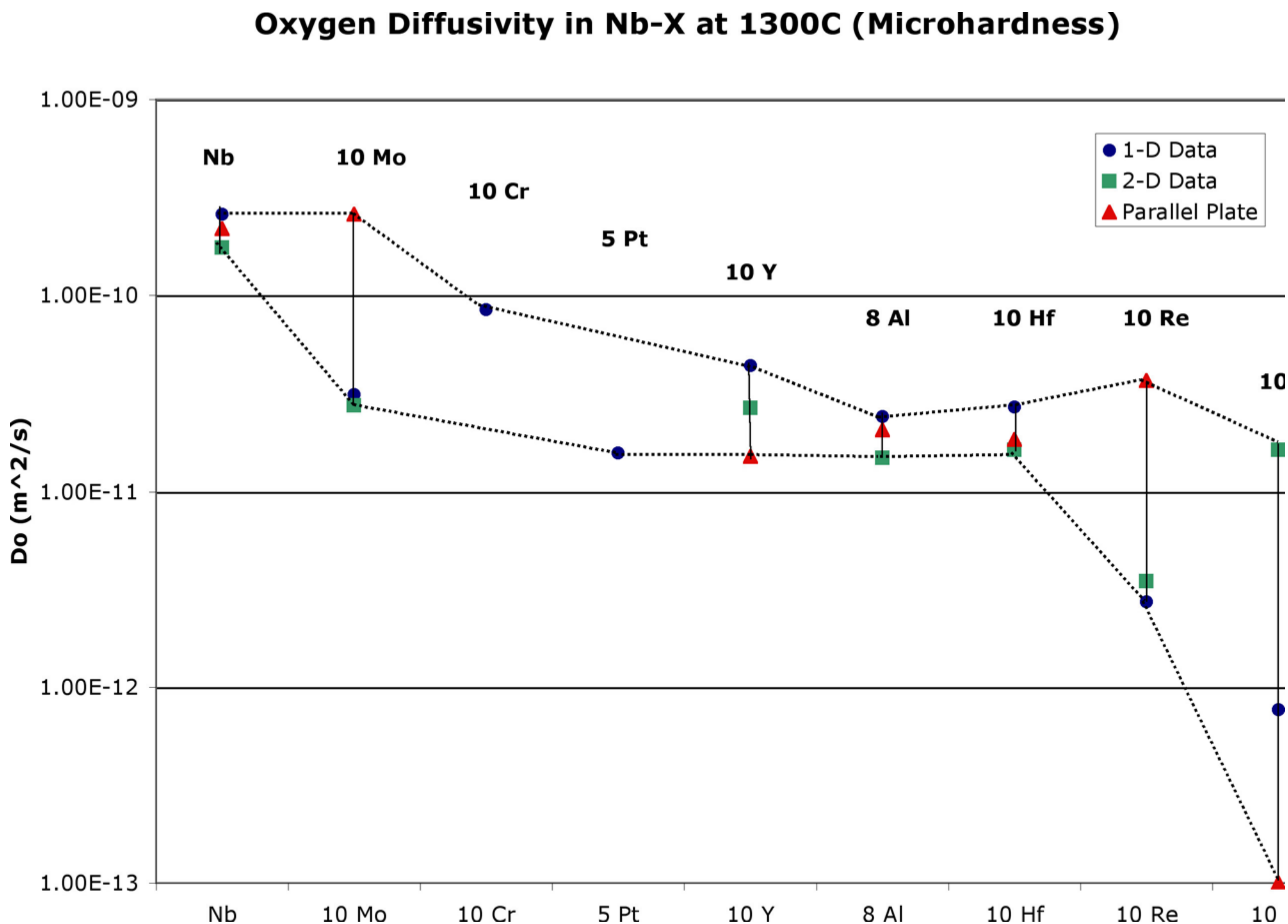


Tie-tetrahedra in the Nb-Pd-Hf-Al quaternary system at 1200˚C

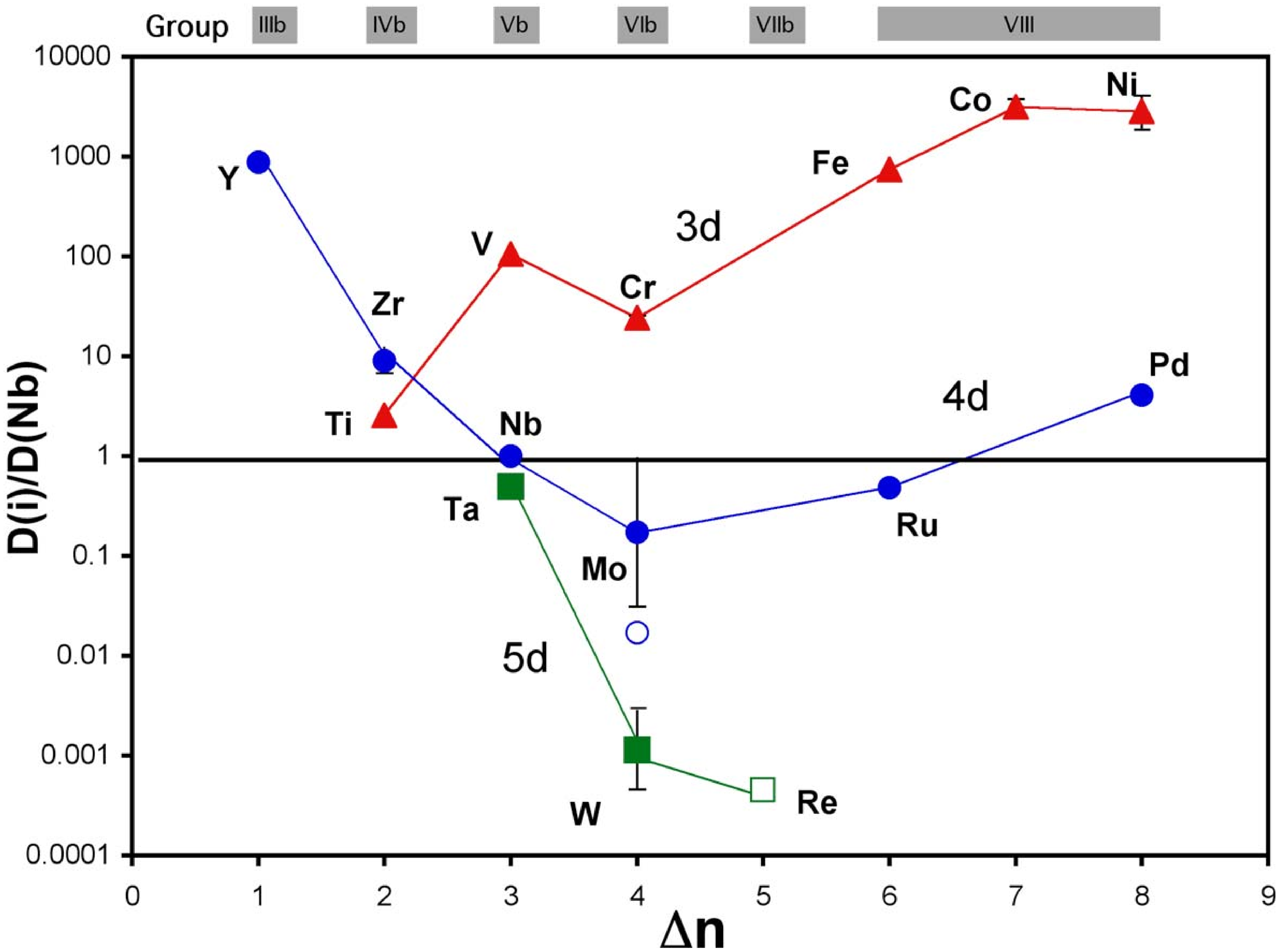


-75
-80
-85
-90
E_f (kJ/mol)
Pd_2HfAl
Pd_2ZrAl
$Pd_2(Hf_{0.75}Zr_{0.25})Al$
$Pd_2(Hf_{0.25}Zr_{0.75})Al$
$(Pd_{0.5}Pt_{0.5})_2HfAl$
$Pt_2(Hf_{0.25}Zr_{0.75})Al$
Pt_2ZrAl
Pt_2HfAl
$Pt_2(Hf_{0.75}Zr_{0.25})Al$
Pt_2HfAl
0.1
0
-0.1
-0.2
-0.3
-0.4
1
0
-1
-2
-3
-4
Energy of Mixing (kJ/mol)
$Pt_2(Hf_{0.25}Zr_{0.75})Al$
$Pd_2(Hf_{0.75}Zr_{0.25})Al$
$Pd_2(Hf_{0.25}Zr_{0.75})Al$
$Pt_2(Hf_{0.75}Zr_{0.25})Al$
$(Pd_{0.5}Pt_{0.5})_2HfAl$
16.6
16.5
16.4
16.3
16.2
16.1
16
15.9
V_a ($\times 10^3$ nm^3)
Pt_2HfAl
Pt_2ZrAl
Pt_2HfAl
$Pt_2(Hf_{0.25}Zr_{0.75})Al$
$Pt_2(Hf_{0.75}Zr_{0.25})Al$
Pd_2ZrAl
$(Pd_{0.5}Pt_{0.5})_2HfAl$
Pd_2HfAl
$Pd_2(Hf_{0.75}Zr_{0.25})Al$
$Pd_2(Hf_{0.25}Zr_{0.75})Al$
0
0.2
0.4
0.6
0.8
1
site fraction Zr, Pt (Y_{Zr}, Y_{Pt})

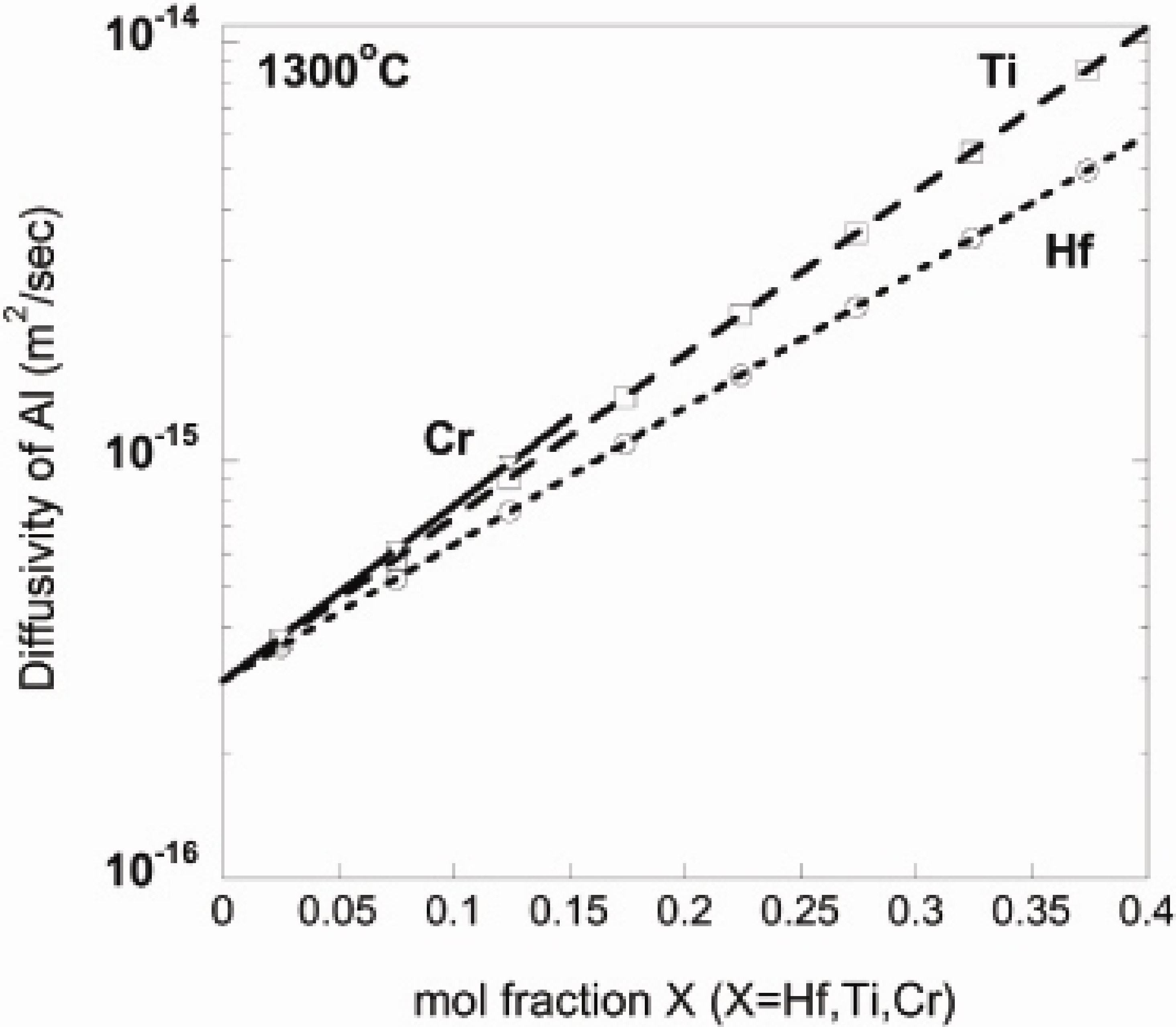

Relative Charge in Octahedral Hole
versus
Metal Sunbstitutional
ρ(M)
ρ(Nb)
1.02
1.00
0.98
0.96
0.94
0.92
Al
Ti
Zr
Nb
Mo
Tc
Ru
Rh
Pd
Hf
W
Re
Os



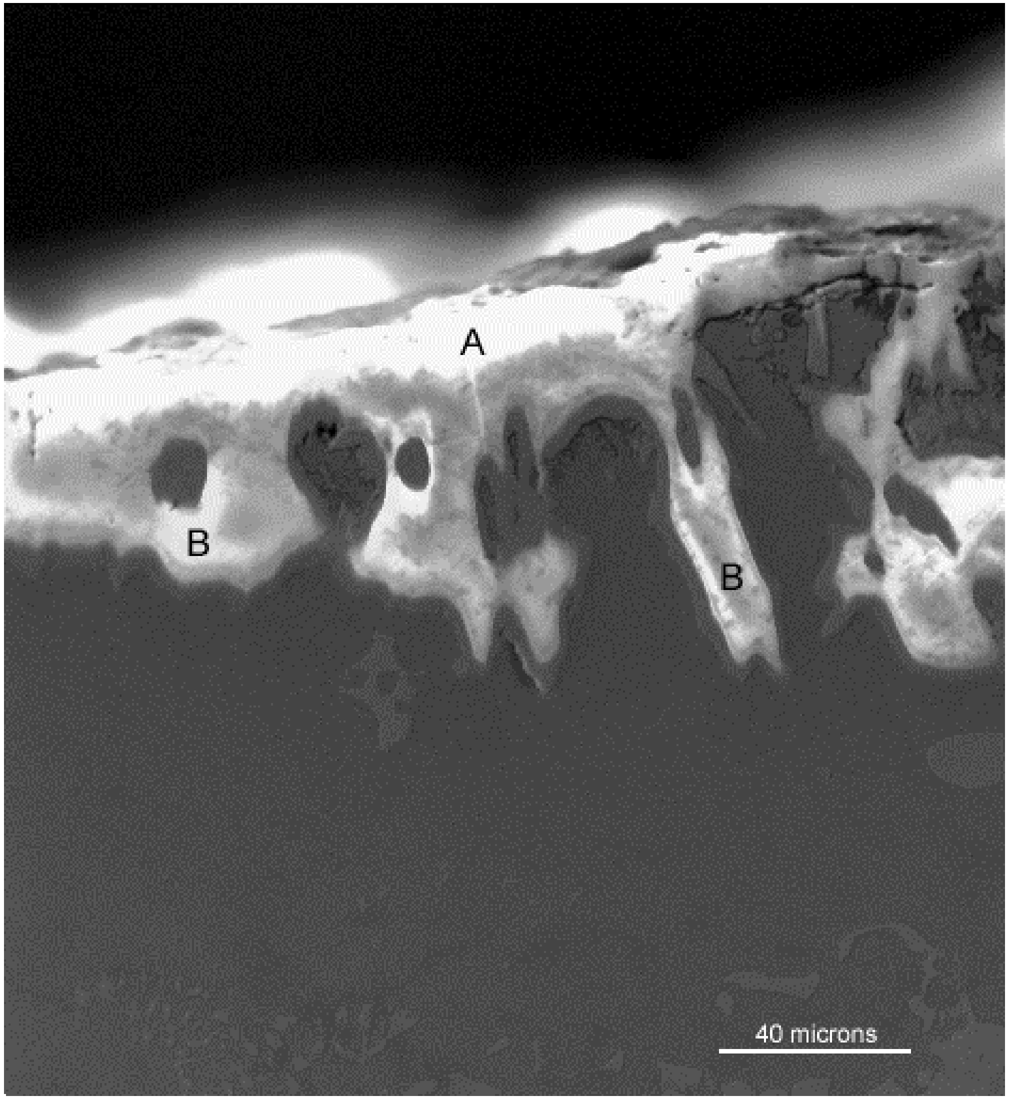
Oxygen Diffusivity in Nb-X at 1300C (Microhardness)
1.00E-09
1.00E-10
1.00E-11
1.00E-12
1.00E-13
Do (m^2/s)
Nb
10 Mo
10 Cr
5 Pt
10 Y
8 Al
10 Hf
10 Re
10
1-D Data
2-D Data
Parallel Plate


Group
IIIb
IVb
Vb
VIb
VIIb
VIII
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
D(i)/D(Nb)
Y
Zr
Ti
V
Nb
Cr
3d
Fe
Co
Ni
Pd
4d
Ru
Ta
Mo
5d
W
Re
0
1
2
3
4
5
6
7
8
9
Δn

Diffusivity of Al in a Nb-X-5Al (in at%) bcc solid solution



Oxide scale in Alloy A’ oxidized at 1300^{o}C



A: Al_2O_3+HfO_2
B: HfO_2

MSc390 Materials Design Projects
Spring 2003

I. **Blastalloy II: LC160 Martensite**

Client: ONR, Dr. Julie Christodoulou
Advisors: Arup Saha; Yana Qian
Team: Dan Cogswell, Joe Dudas, Ken Liu

II. **Blastalloy III: PH-TRIP Austenite**
Client: ONR, Dr. Julie Christodoulou
Advisors: Dr. Su Hao; Zhe Liu
Team: Danijel Gostovic, Sai-Pong Leung, Derek Norton

III. **Dragonslayer II: Carburizing Stainless Bearing Steel (CS62+)**
Client: DOE-OIT, P&W, QuesTek
Advisors: Dr. Jay Gao; Ben Tiemens
Team: Loren Darling, Thor Gudmundsson

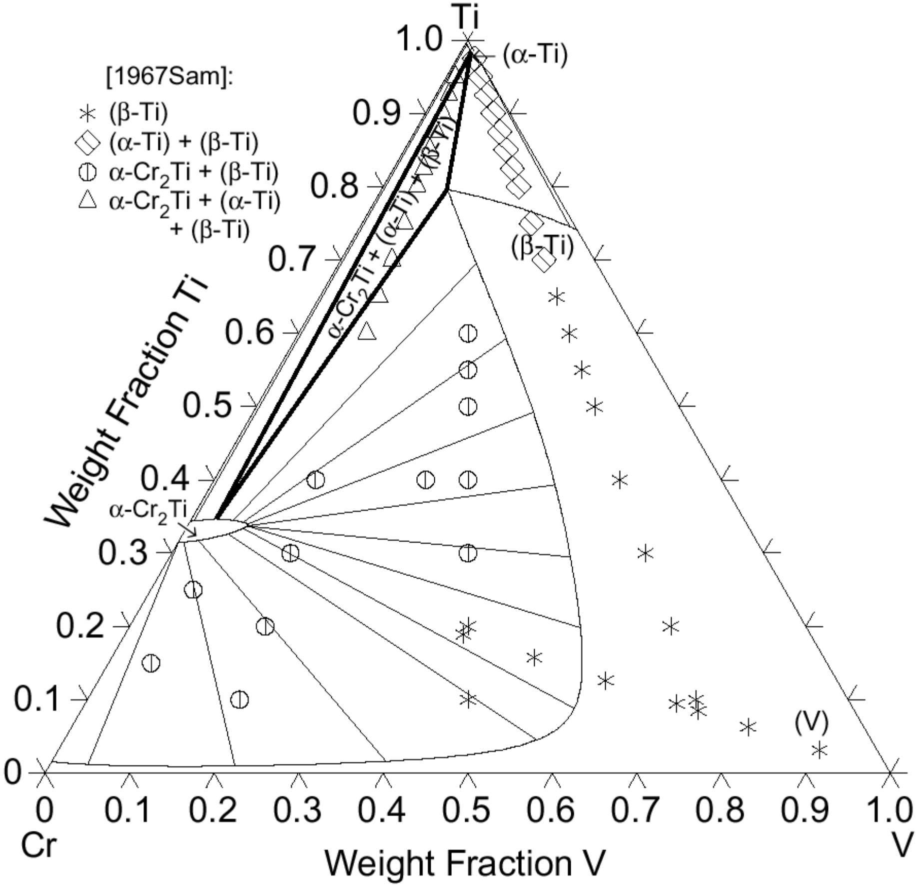
IV. **MX4: Ni Aeroturbine Blade Alloy**
Client: NSF-FRG (OSU), P&W, GEAE
Advisors: Dr. Gautam Ghosh; Chandler Becker
Team: Travis Harper, Mike McCarren, Paul Von Dollen

V. **Noburnium: Nb Superalloy**
Client: AF-MEANS, Dr. Craig Hartley
Advisors: Abhijeet Misra; Dave Bryan
Team: Erhan Altinoglu, Jennifer Bolos, Nora Colligan

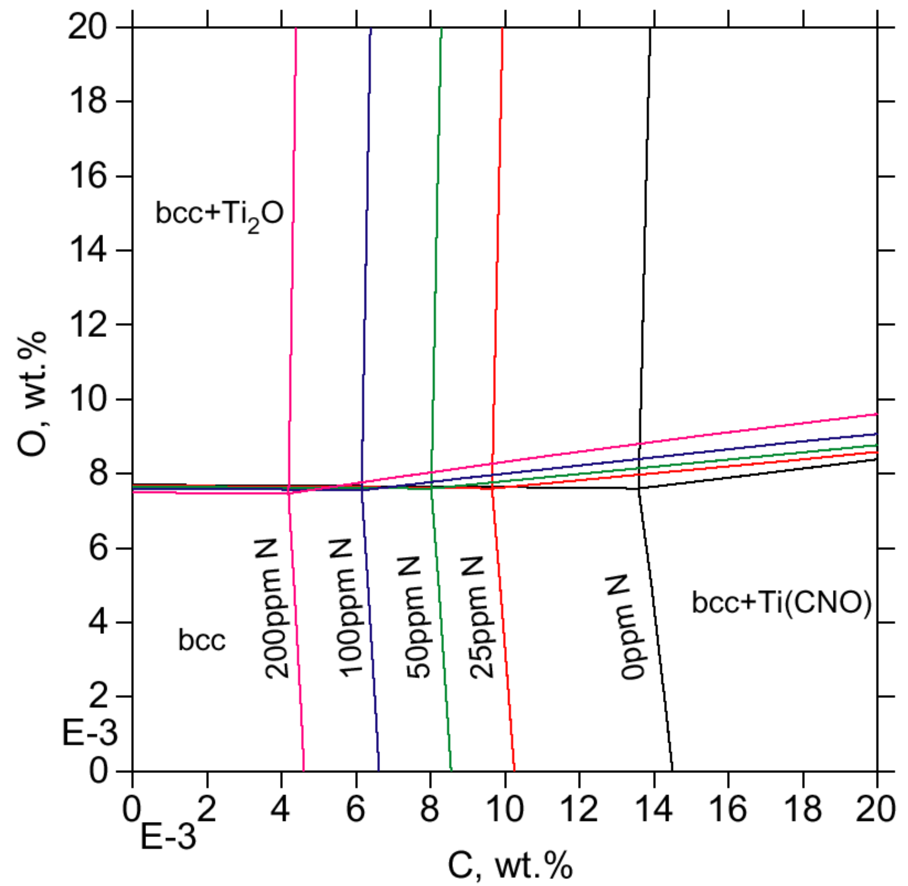
VI. **Terminator 4: FrankenSteel Goes to Mars (Biomimetic Self-Healing Alloy Composite)**
Client: NASA-Houston, Dr. Brad Files
Advisors: Jin-won Jung; Michele Manuel
Team: Wendy Cheng, Steve Knapp, Richard Scheunemann

VII. **HT Aluminum/Bulk Metallic Glass**
Client: DARPA-SAM, Boeing, P&W, QuesTek
Advisors: Ryan Rathbun; Keith Knipling
Team: Bryan Harder, Nik Hrabe, Alison Markowitz

V-Cr-Ti Alloys



Isothermal Section at 600°C



Solubility Limits of C and O in V-4.1Cr-4.3Ti at 1000°C

Paradigm Shifts: MSE Integration

a) discovery based → design based
- downstream cost of discovery

b) empirical → mechanistic/predictive

c) statistical (eng.)
deterministic (sci.) $\Big\}$ **→ probabilistic**

- prediction of multiple properties from defect distribution functions

- designed variation (predictive robust design: performance/variation tradeoff)

d) computational mat. sci. (toys) → computational mat. eng. (tools)

e) reductionist analytical → holistic (systems) synthetic

Optimal Integration:
Tactical science in support of strategic engineering