Fall 10-3-2012

From Genome to Flying Cyberalloys: The First Half Century

G. B. Olson
Northwestern University

From Genome to Flying Cyberalloys: The First Half Century

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NORTHWESTERN UNIVERSITY

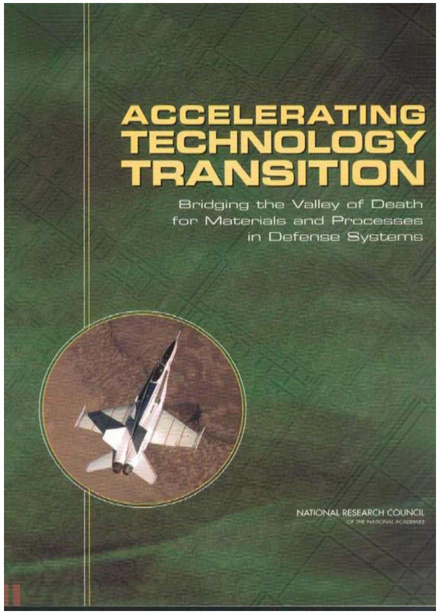
QUESTEK INNOVATIONS LLC

Materials Genome Initiative
for Global Competitiveness

June 2011

Fundamental databases and tools enabling reduction of the 10-20 year materials creation and deployment cycle by 50% or more.

National Science and Technology Council (NSTC)/ Office of Science and Technology Policy (OSTP)



NRC 2004

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

Chapter 3, p. 42:

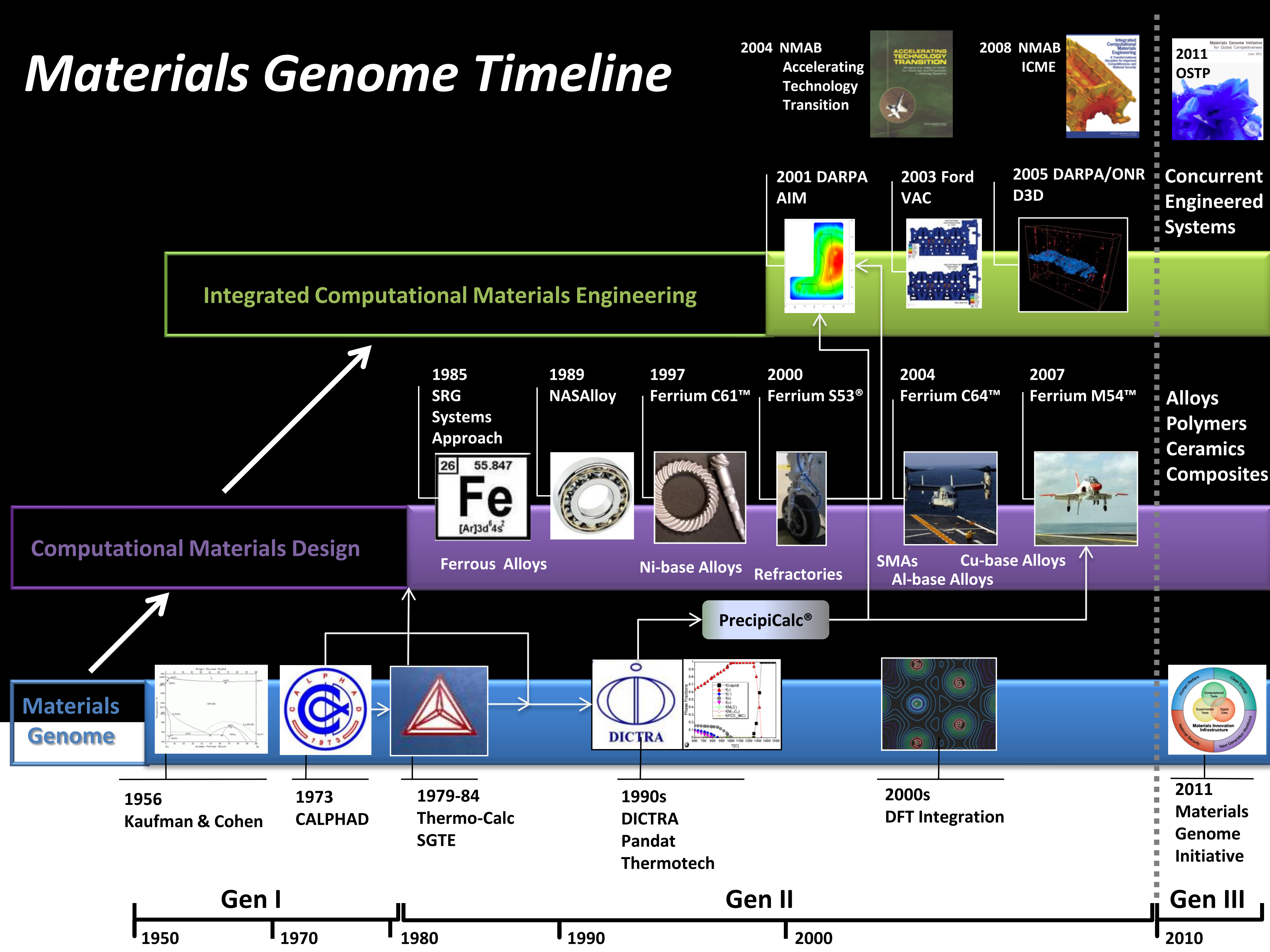
A productive model may be the health-driven research system operated by the National Institutes of Health, spanning the full range from molecular biology to medicine. While the academic value system of the physical sciences has generally suppressed the creation of engineering databases, the life sciences have forged ahead with the **Human Genome project** representing the greatest engineering database in history. A parallel **fundamental database initiative** in support of computational materials engineering could build a physical science/engineering link as effective as the productive life science/medicine model.

Recommendation : The *Office of Science and Technology Policy* should lead a national, multiagency initiative in computational materials engineering to address three broad areas: methods and tools, databases, and dissemination and infrastructure.

First Flight: QuesTek *Ferrium* S53®
T-38 main landing gear piston
December 17, 2010

Material approval:	**November 2009**
Component approval:	**August 2010**
Component installation:	**November 2010**
First flight:	**December 2010**

QuesTek®
INNOVATIONS LLC


Materials Genome Timeline
2004 NMAB Accelerating Technology Transition
ACCELERATING TECHNOLOGY TRANSITION
2008 NMAB ICME
2011 OSTP
Concurrent Engineered Systems
2001 DARPA AIM
2003 Ford VAC
2005 DARPA/ONR D3D
Integrated Computational Materials Engineering
1985 SRG Systems Approach
26 55.847 Fe [Ar]3d6 4s2
1989 NASAlloy
1997 Ferrium C61™
2000 Ferrium S53®
2004 Ferrium C64™
2007 Ferrium M54™
Alloys
Polymers
Ceramics
Composites
Computational Materials Design
Ferrous Alloys
Ni-base Alloys
Refractories
SMAs
Cu-base Alloys
Al-base Alloys
PrecipiCalc®
Materials Genome
DICTRA
1956 Kaufman & Cohen
1973 CALPHAD
1979-84 Thermo-Calc SGTE
1990s DICTRA Pandat Thermotech
2000s DFT Integration
2011 Materials Genome Initiative
Gen I
Gen II
Gen III
1950
1970
1980
1990
2000
2010

MTL/SRG

A) Cybersteels (ONR,DARPA D3D; AM)
B) HT Carburizing Steels (DOE-OIT; GM)
C) Cyberalloys/SMA (NASA, ONR, DARPA, MDT, GM, Ford/Boeing)
D) Bulk Metallic Glasses (DARPA-SAM, ONR)

GOVERNMENT

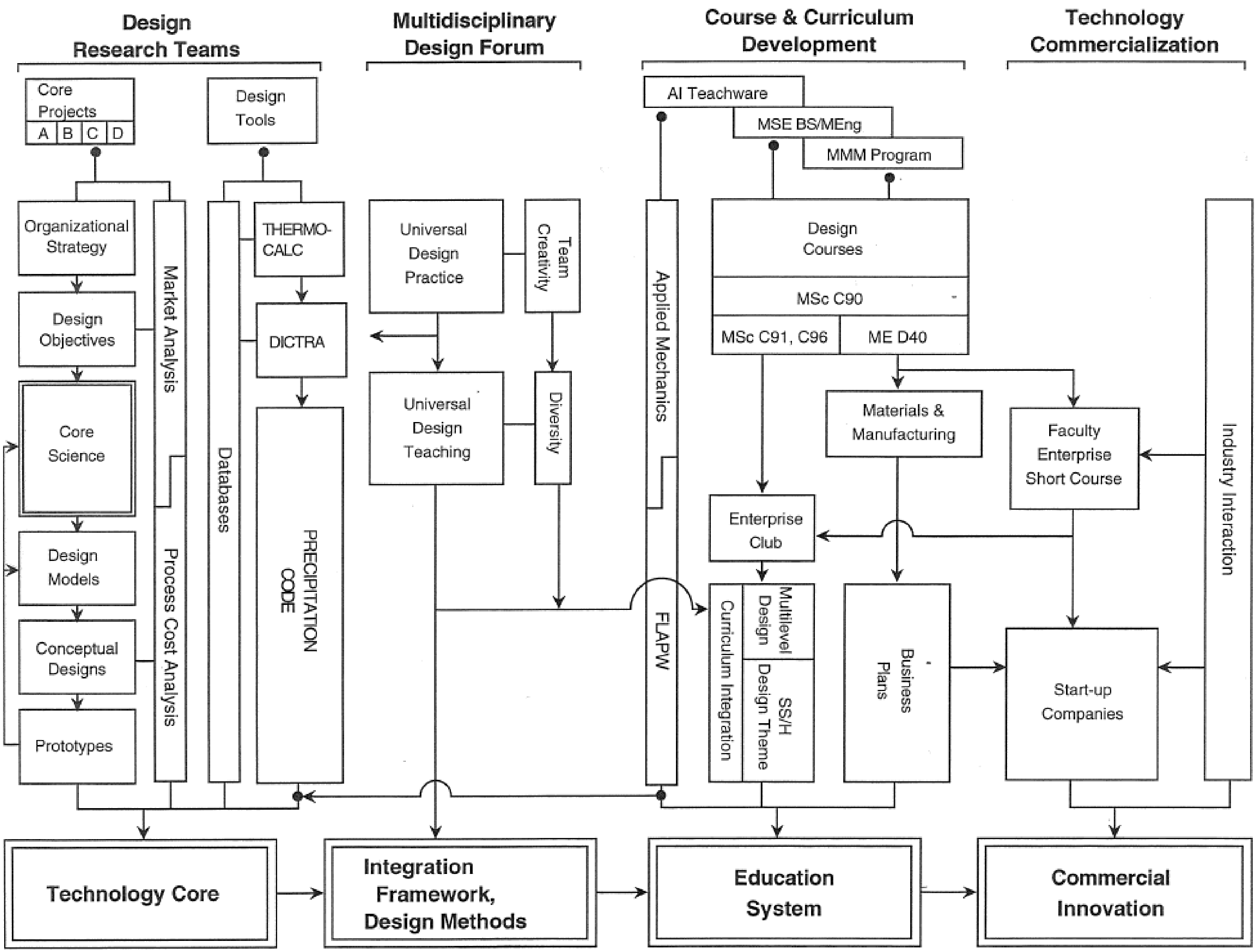
NAWC/AD	A	Lee
NRL	A	Spanos, Rowenhorst, Fonda
ARL/WMD	B	Montgomery, Mathaudhu
AFRL	C,D	Woodward, Miracle, Simmons
FLORIDA	C	Manuel
LEHIGH	C	Harlow
WISCONSIN-MAD	C,D	Perepezko
IIT	C,D	Nash

UNIVERSITY

NORTHWESTERN	A,B,C,D	Olson, Freeman, Brinson, Isheim, Chen, Jerome, Espinosa, Liu, Fine, Voorhees; High Resolution Microanalysis
GIT	A	McDowell
UCSB	A	Pollock
CSM	A,C	Eberhart
OHIO STATE	A,C	Fraser, Mills, Lippold, Babu
MIT	A,D	Parks
WPI/CHTE	B	Apelian, Backman
PURDUE-CALUMET	B	Abramowitz
KTH (Stockholm)	C	Agren, Borgenstam

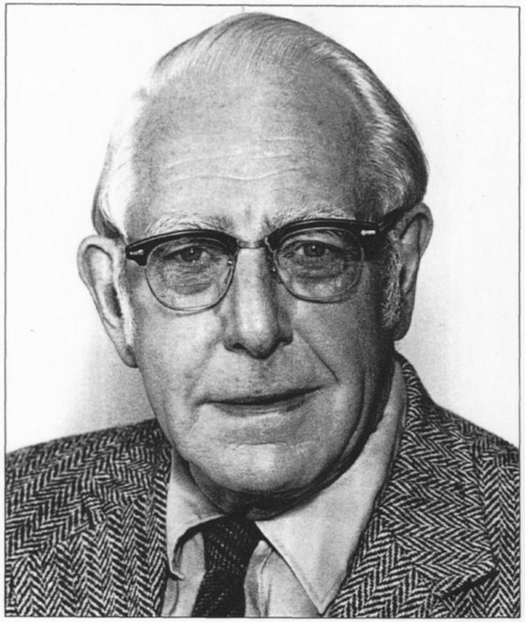
INDUSTRY

QUESTEK	A,B,C,D	Kuehmann, Feinberg, Huang, Li, Sassaman, Backs, Grabowski, Jou, Misra, Sebastian, Counts, Hamann, Kern, Prasanna, Wright
ARCELOR-MITTAL	A	Bhattacharya, Yakubovsky
LATROBE STEEL	A,B	Tomasello, Balliett
CATERPILLAR	A,B	Chen, Johnson, Sherman
ALLVAC STEEL	A,B	Lippard
SFTC	A	Bandar
GM	B, C	Sachdev, Sarosi
FORD	B,C	Li, Sherman
BOEING	C,D	Bowden, Sankaran
PRATT & WHITNEY	B,C,D	Fowler, Schirra, Watson
MEDTRONIC	C	Adler
HOWMET	D	Wolter



Design Research Teams
Multidisciplinary Design Forum
Course & Curriculum Development
Technology Commercialization
Core Projects
A B C D
Design Tools
AI Teachware
MSE BS/MEng
MMM Program
Organizational Strategy
Market Analysis
Databases
THERMO-CALC
Universal Design Practice
Team Creativity
Applied Mechanics
Design Courses
MSc C90
MSc C91, C96
ME D40
Design Objectives
DICTRA
Core Science
PRECIPITATION CODE
Universal Design Teaching
Diversity
Materials & Manufacturing
Faculty Enterprise Short Course
Industry Interaction
Enterprise Club
Design Models
Process Cost Analysis
FLAPW
Curriculum Integration
Multilevel Design
SS/H Design Theme
Business Plans
Conceptual Designs
Start-up Companies
Prototypes
Technology Core
Integration Framework, Design Methods
Education System
Commercial Innovation

STRUCTURE- C.S. Smith



INTERACTIVE HIERARCHY

- -Space-Filling Aggregates: materials science, biology, geology
- -Perfection/Imperfecton
- -Entity/Identity
- -"Mesoscopic" Regime

} duality of description

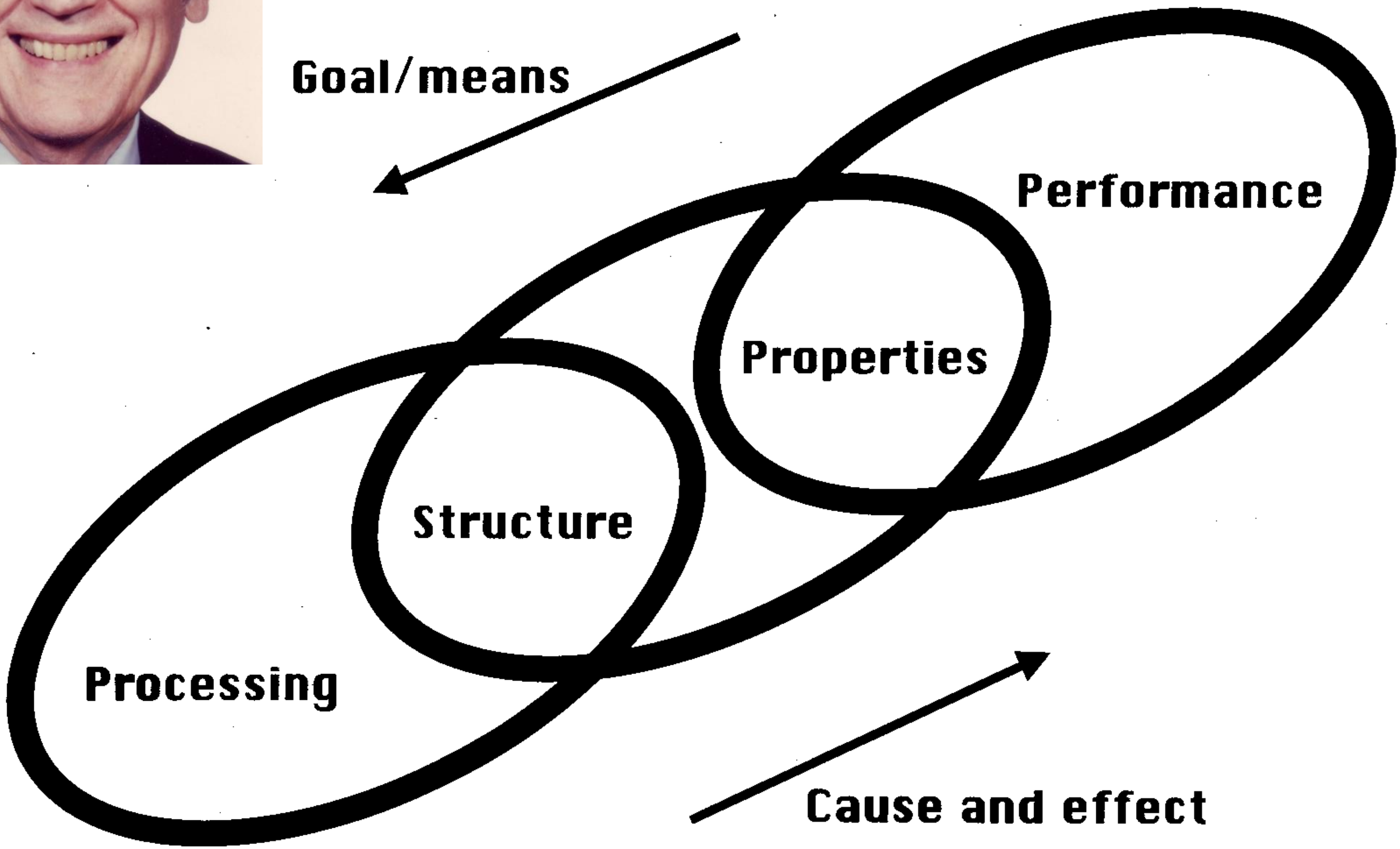
REAL COMPLEXITY VS. IDEALIZED SIMPLICITY

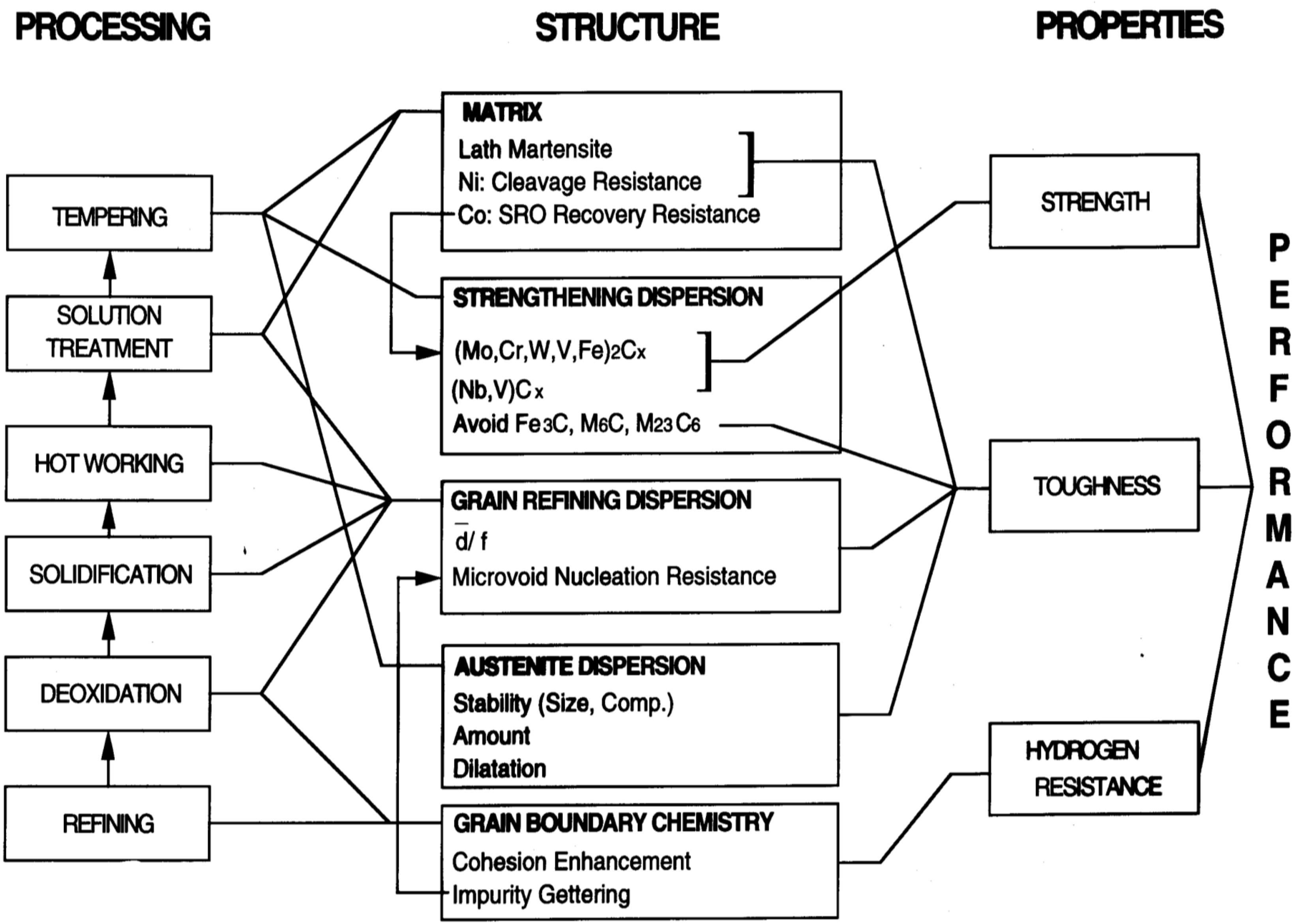
- -Cartesian Corpuscular Philosophy
- -Atom/Continuum

DYNAMICS

- -Spatial and Temporal Hierarchy: Smith/Zener
- -Nonequilibrium
- -Path (History) Dependence

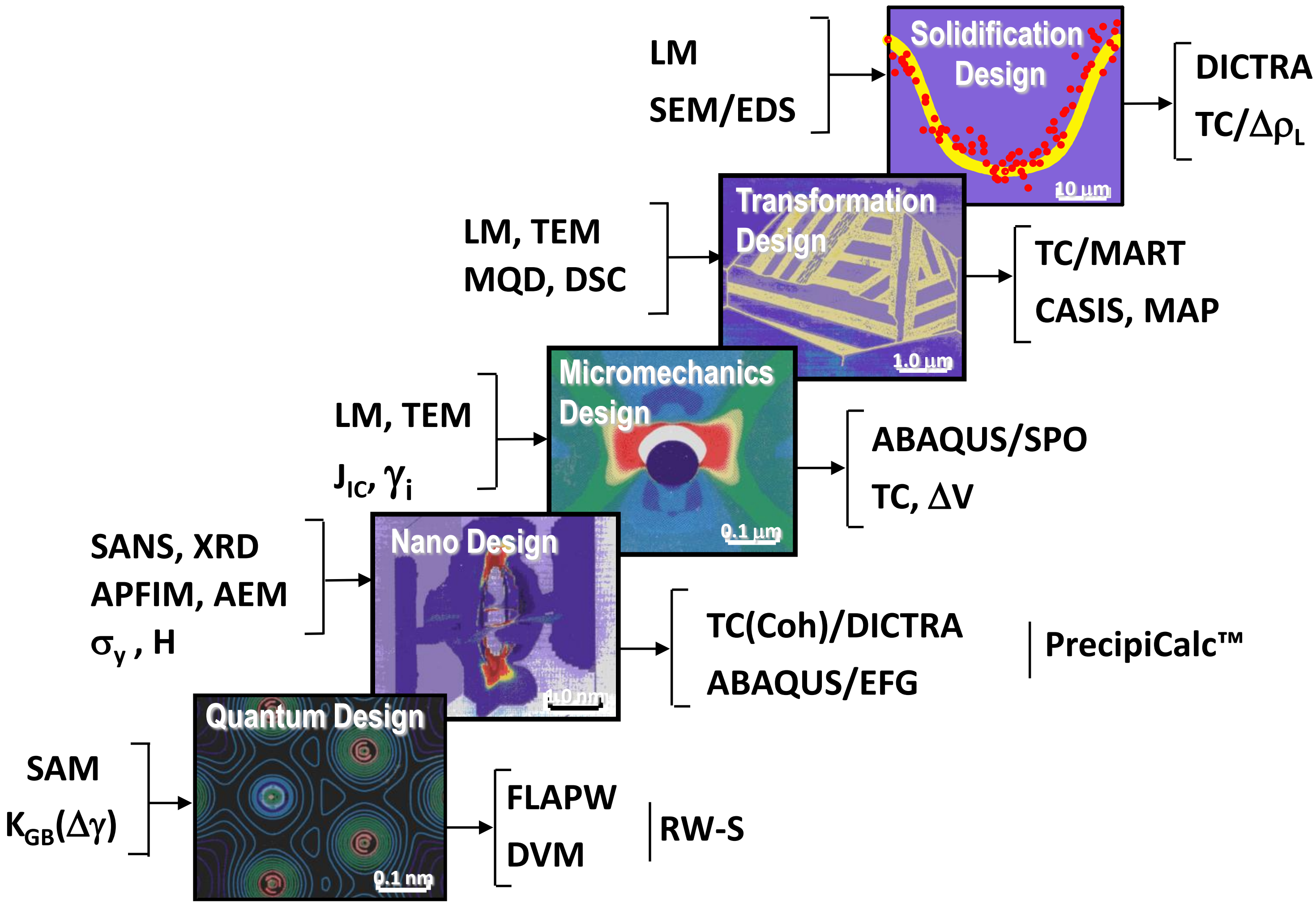
Cohen's Reciprocity



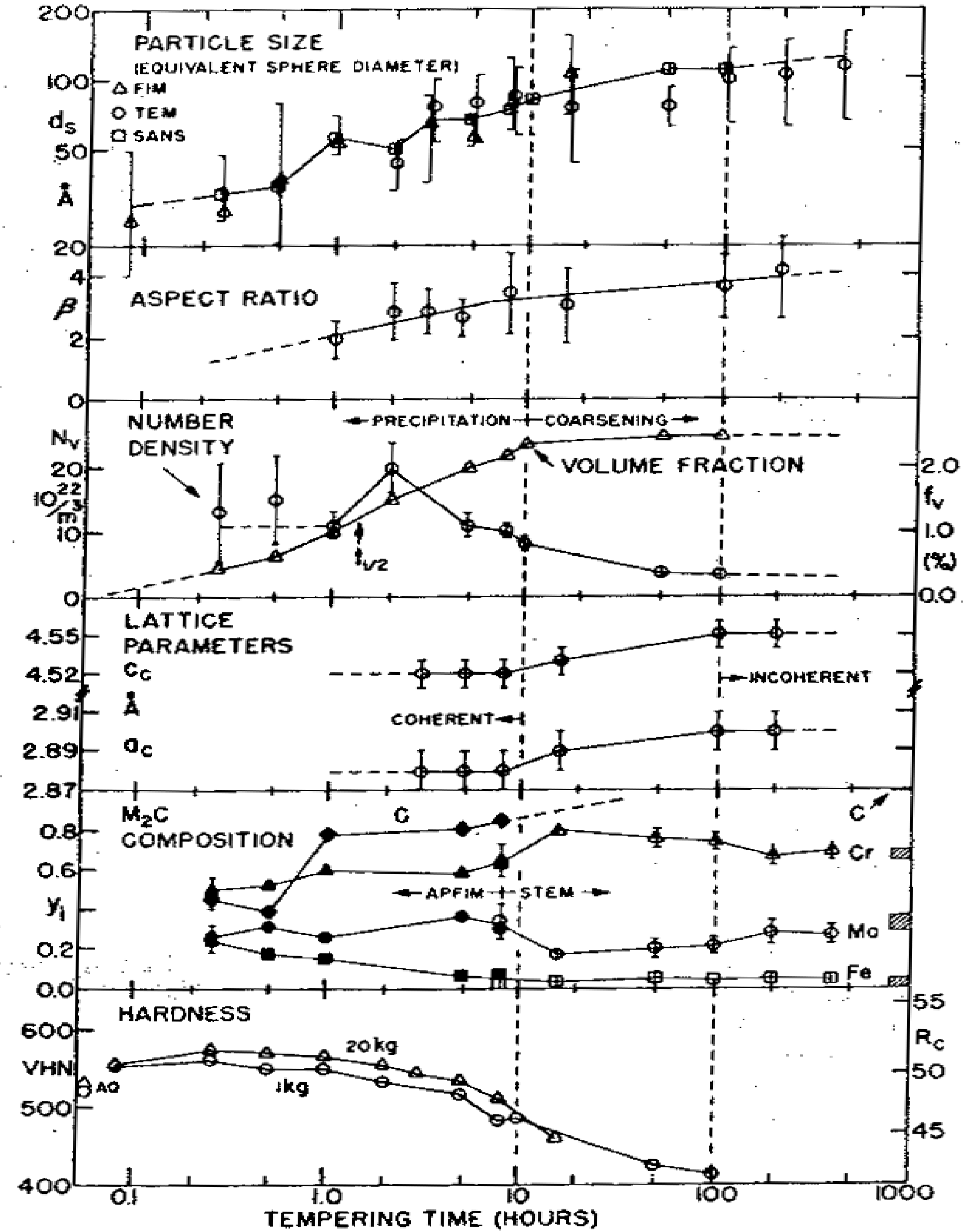


PROCESSING
STRUCTURE
PROPERTIES
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
TEMPERING
STRENGTH
STRENGTHENING DISPERSION
SOLUTION TREATMENT
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
HOT WORKING
GRAIN REFINING DISPERSION
TOUGHNESS
d/ f
SOLIDIFICATION
Microvoid Nucleation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

Hierarchy of Design Models

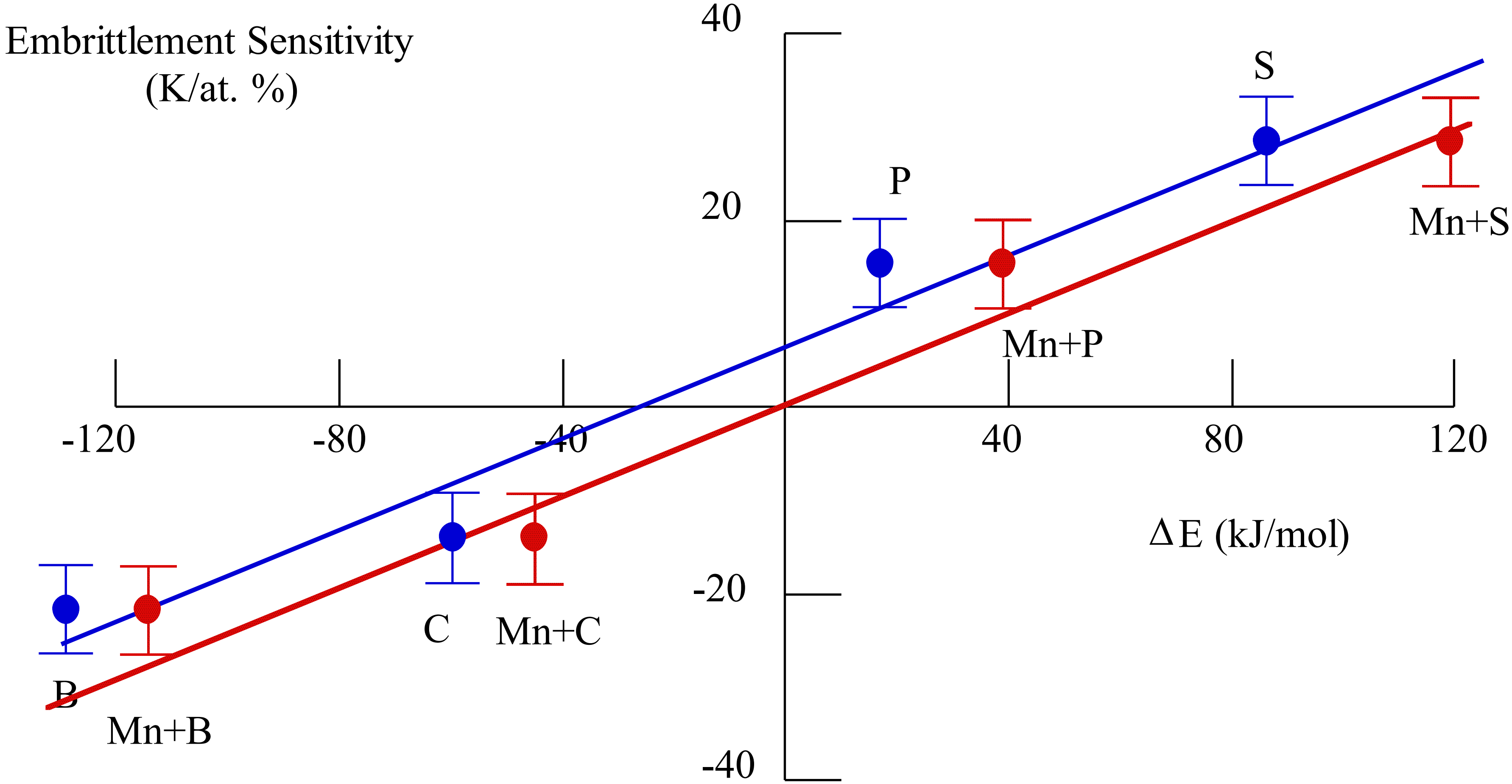


M2C Precipitation

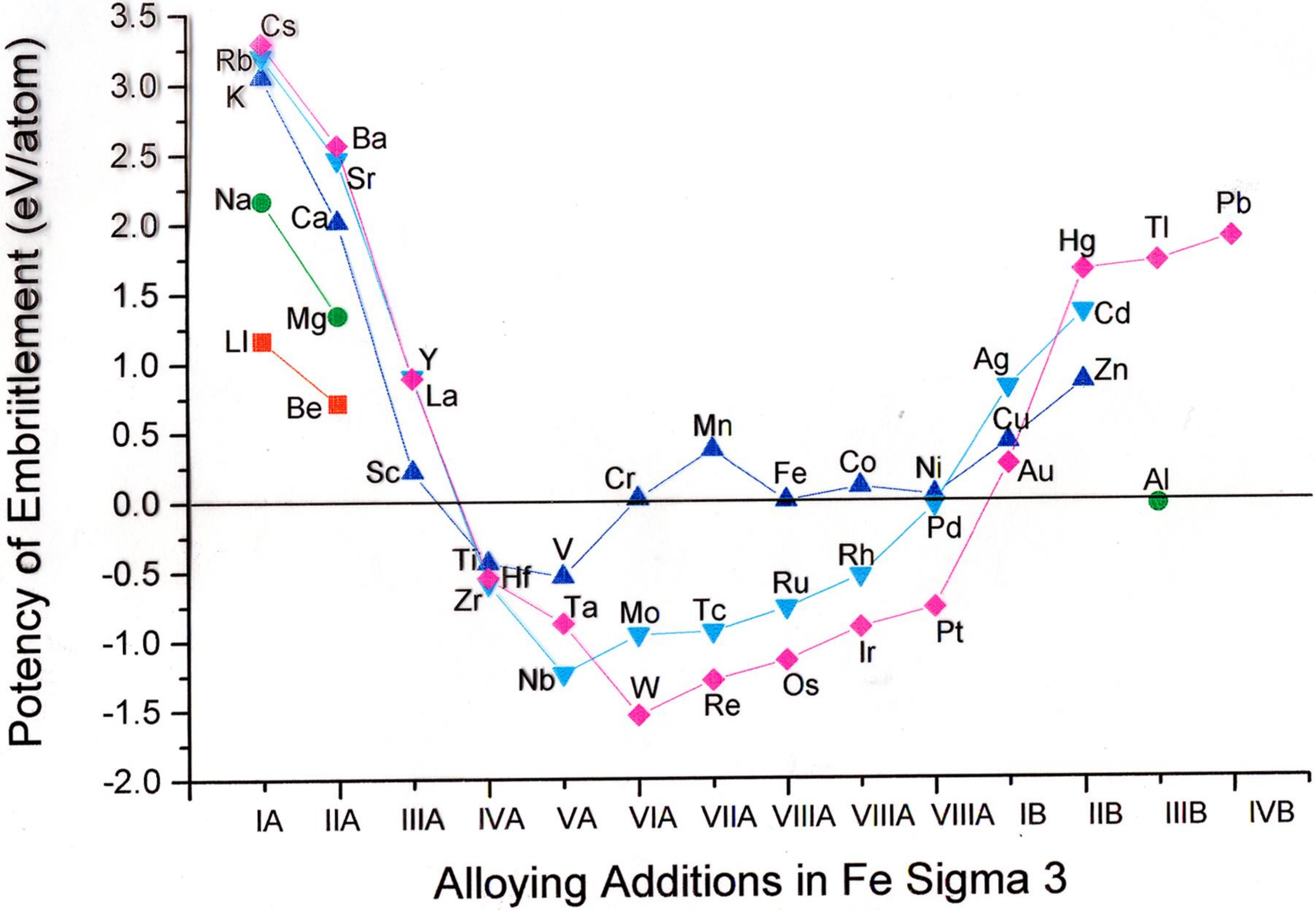


M2C carbide precipitation behavior in AF1410 steel vs. tempering time at 510C following 1 hour solution treatment at 830C

Grain Boundary Embrittlement



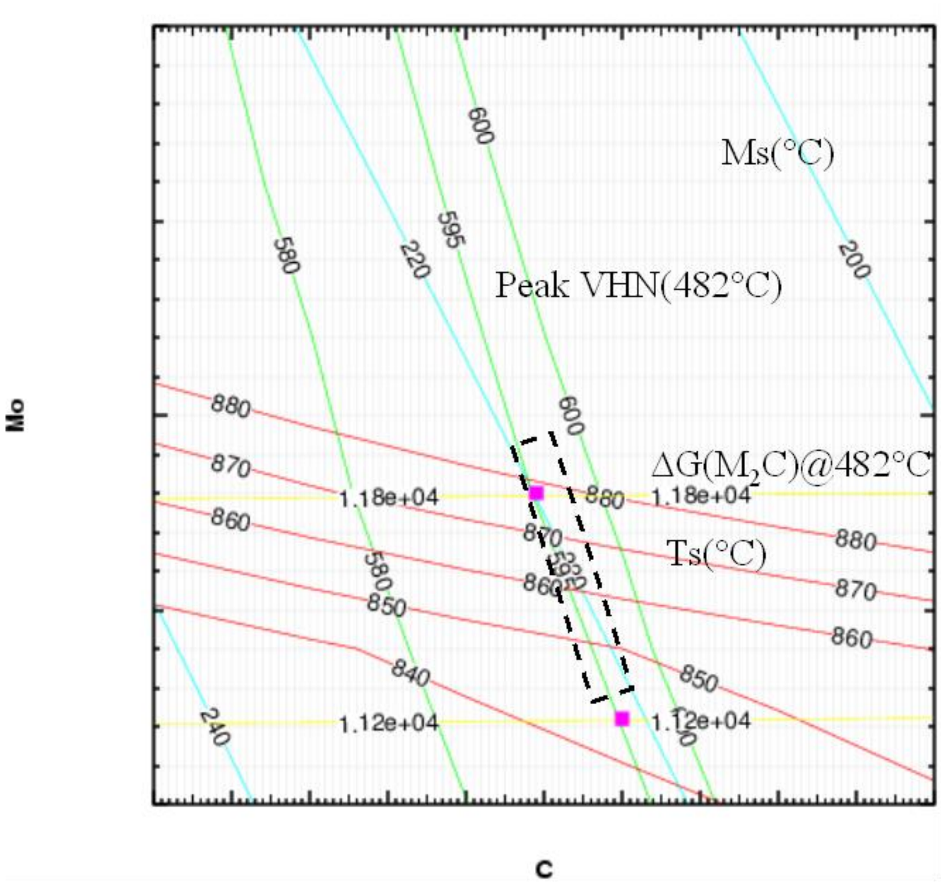
J.R. Rice and J.-S. Wang, Mater. Sci. Eng., 1988



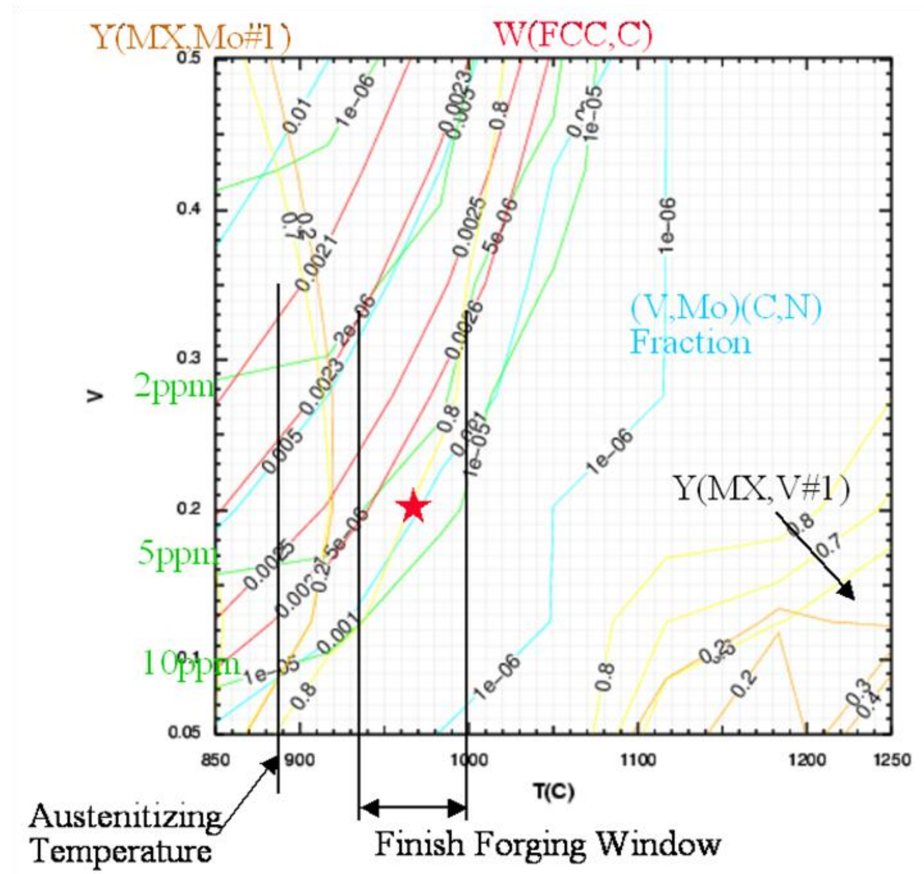
Potency of Embrittlement (eV/atom)
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Cs
Rb
K
Ba
Sr
Na
Ca
Mg
LI
Be
Y
La
Sc
Ti
Hf
Zr
V
Ta
Nb
Cr
Mo
W
Mn
Tc
Re
Fe
Ru
Os
Co
Rh
Ir
Ni
Pd
Pt
Ag
Cu
Au
Hg
Cd
Zn
Tl
Al
Pb
IA
IIA
IIIA
IVA
VA
VIA
VIIA
VIIIA
VIIIA
VIIIA
IB
IIB
IIIB
IVB
Alloying Additions in Fe Sigma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

Example: Design Integration with CMD

Matrix + Strengthening Dispersion Design



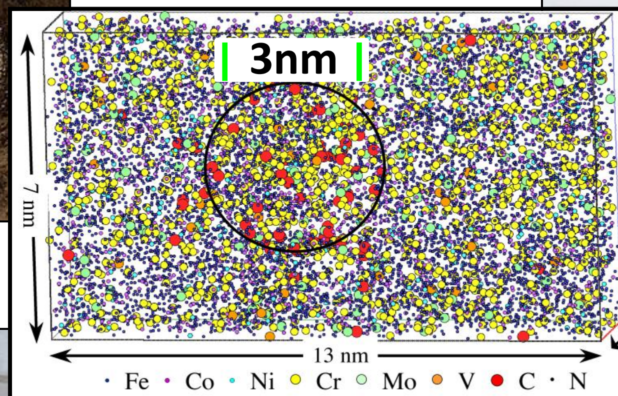
Grain Pinning Dispersion Design



CyberSteels to Market

Ferrium C61 **AMS6517**

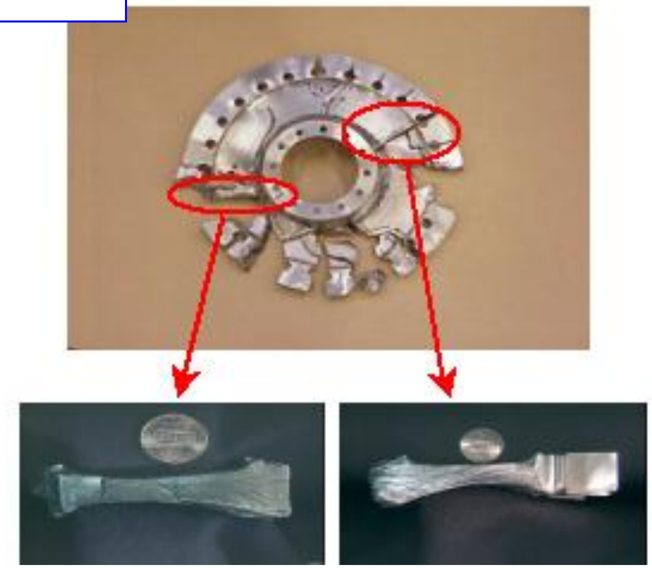
Ferrium C64 **AMS6509**

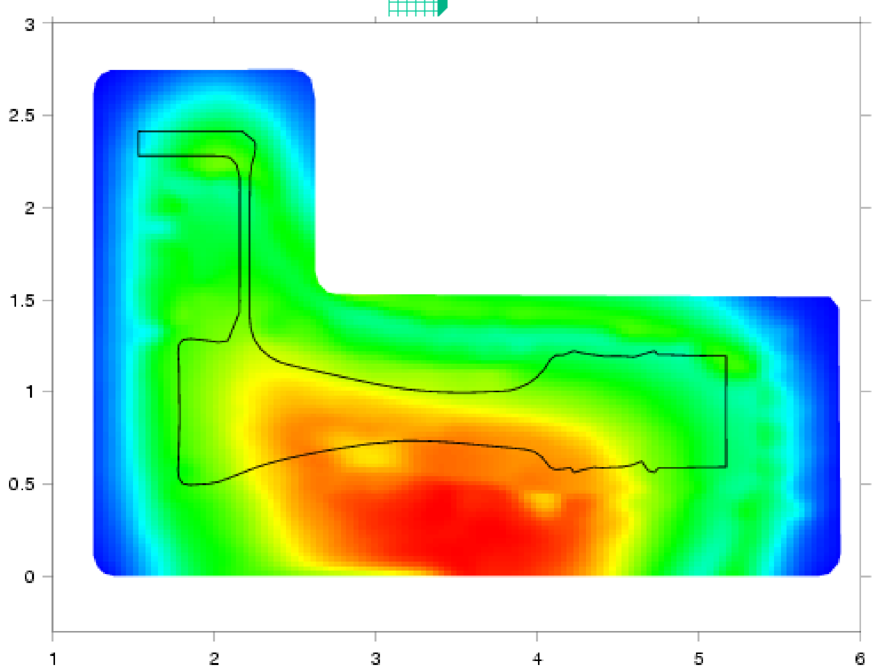


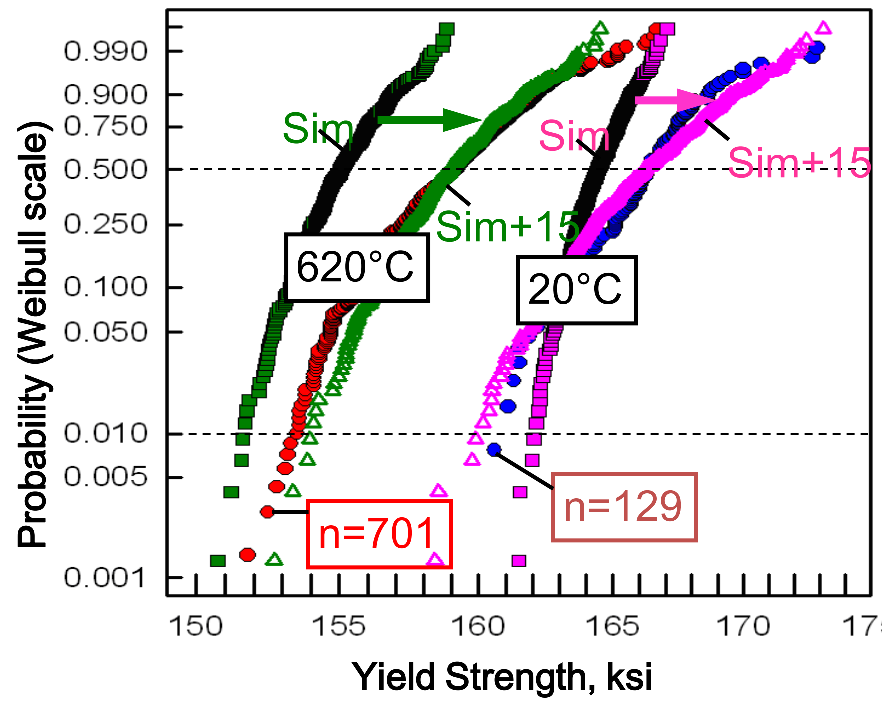
Ferrium S53 Stainless **AMS5922**

Ferrium M54 **AMS6516**

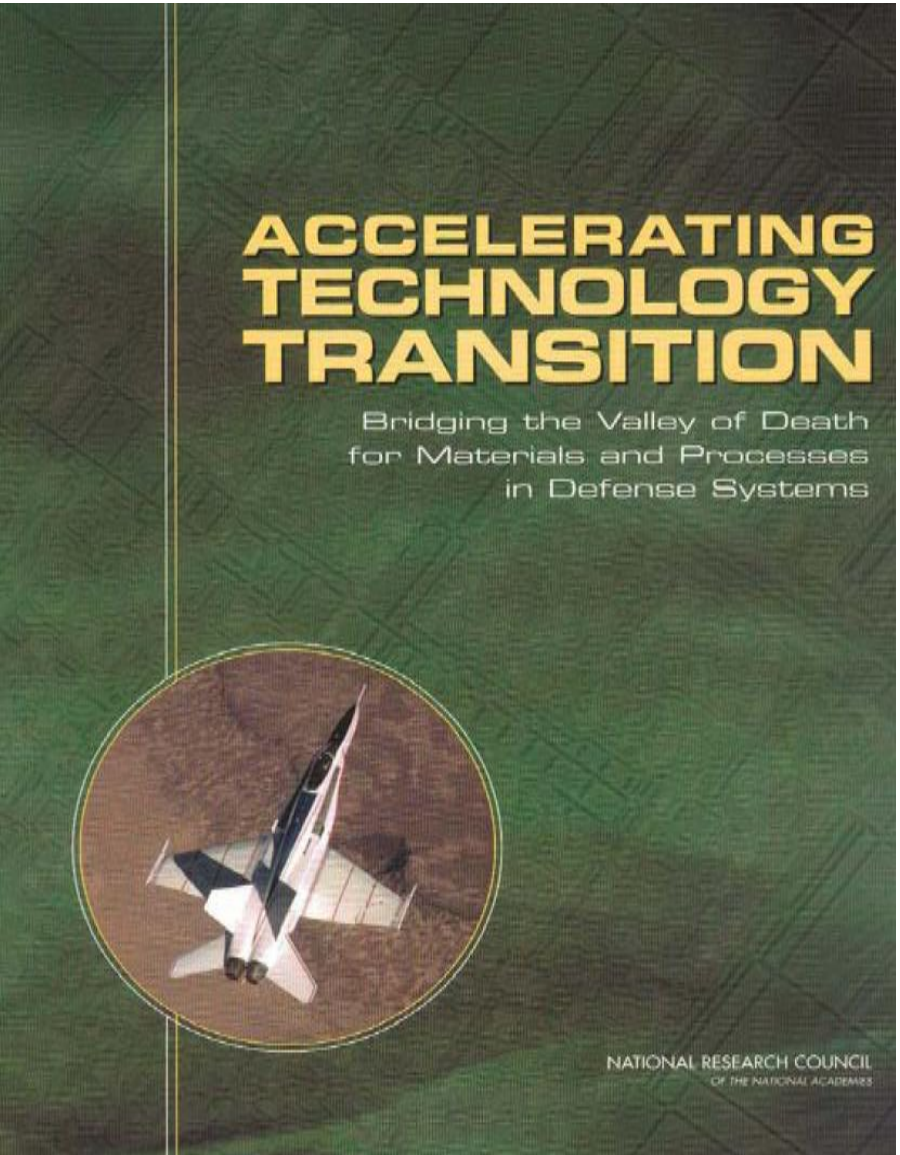

DARPA
AIM
Accelerated Insertion of Materials
Documentum
eMatrix
Oracle
Microsoft Access
Work Flow
Information Repository
Exploration Tech.
iSIGHT
Analysis
Networking
DRM
Java/HTML
LSF/Java
Geometric Modeling
Structural Modeling
Thermal Modeling
Gamma Prime Model
Gamma Prime Model
Microsoft Excel
EDS
ANSYS
ANSYS
MSC SOFTWARE
DEFORM
PrecipiCalc
QuesTek
INNOVATIONS LLC




3
2.5
2
1.5
1
0.5
0
1
2
3
4
5
6


Probability (Weibull scale)
0.990
0.900
0.750
0.500
0.250
0.100
0.050
0.010
0.005
0.001
Sim
Sim+15
Sim
Sim+15
620°C
20°C
n=701
n=129
150
155
160
165
170
175
Yield Strength, ksi

NRC 2004



NRC 2008: Integrated Computational Materials Engineering

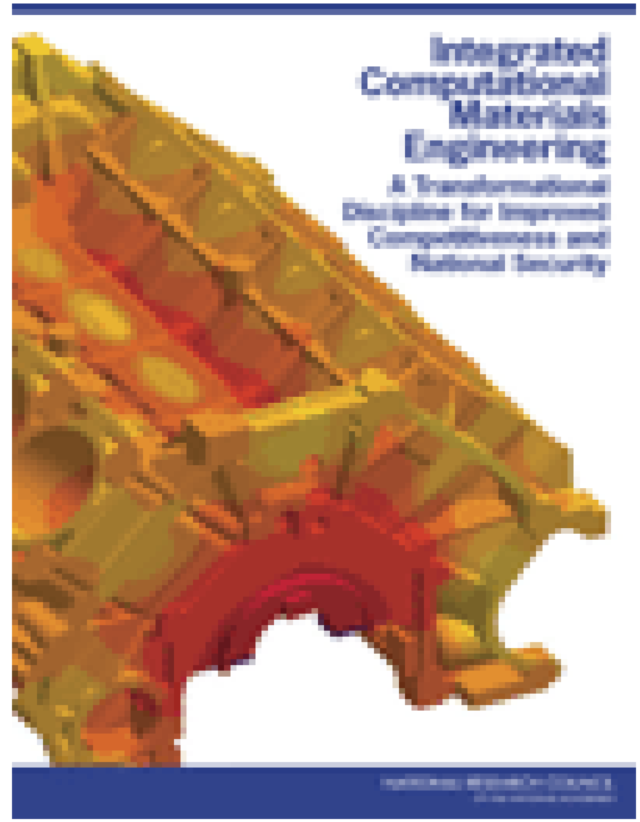
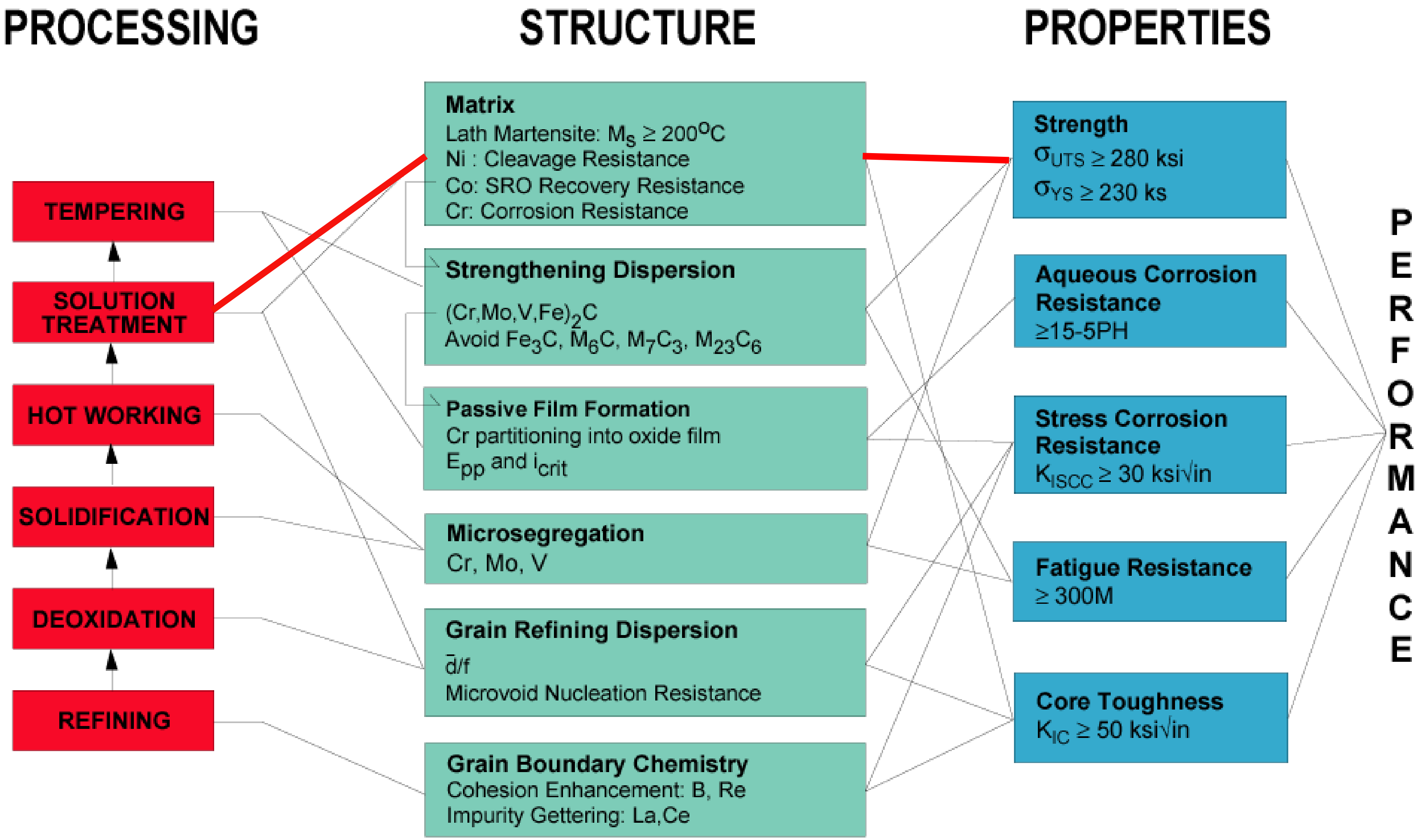


TABLE 3.1 Some Computational Materials Engineering Tools

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

S53 System Flow-Block Diagram



S53 Robust Design Sensitivity Analysis

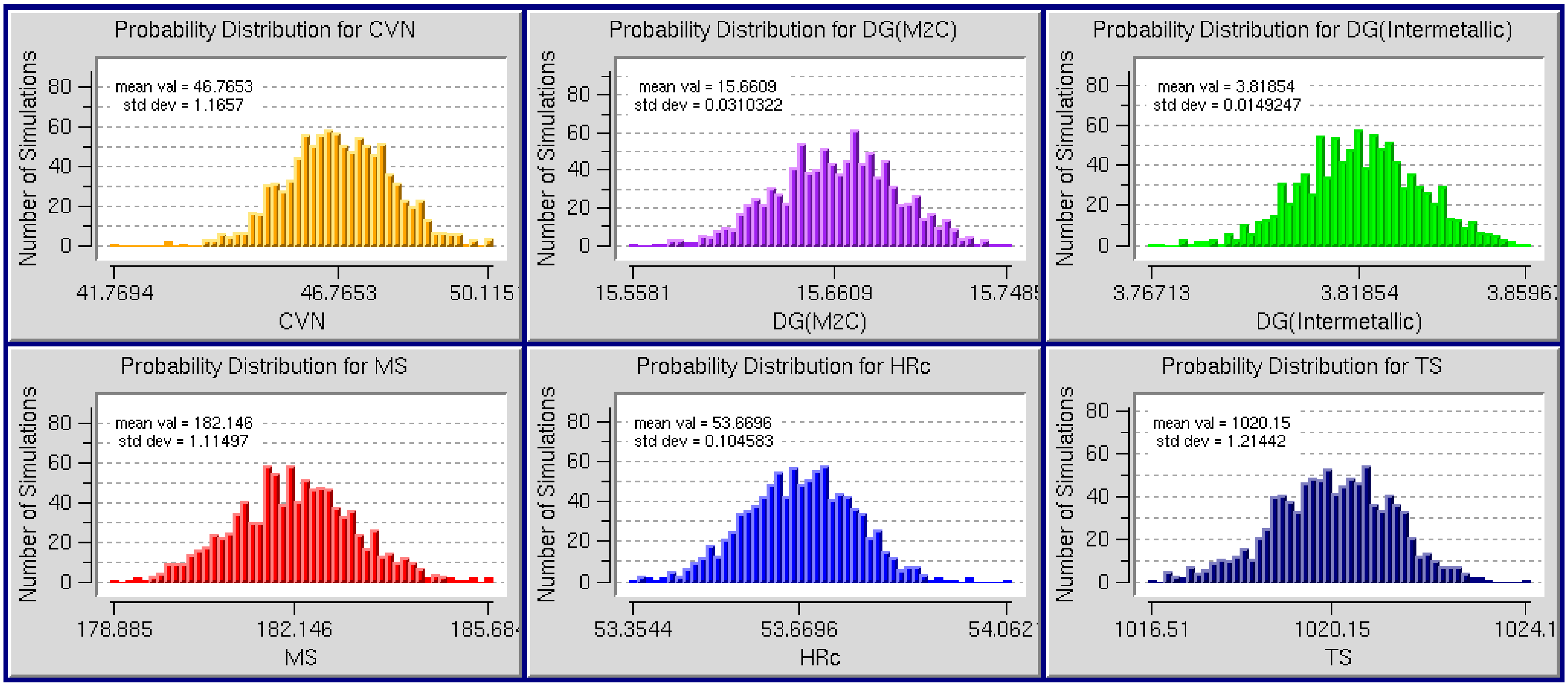
Compositional Variations (wt%, ±6σ):

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

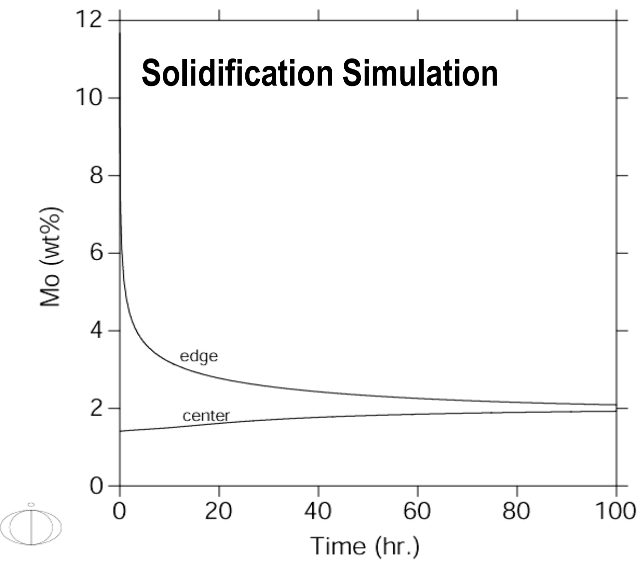
CMD/ iSIGHT

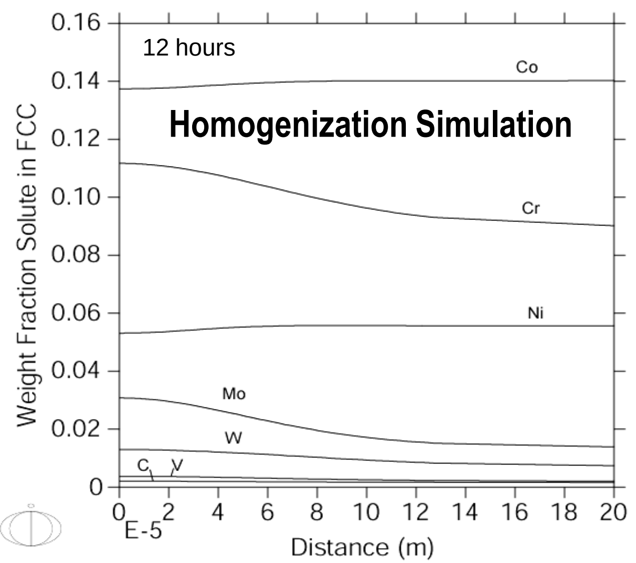
Variations of:
Structure — carbide solvus Ts**,** martensite Ms, precipitation control ΔG's
Property — hardness HRc, toughness CVN

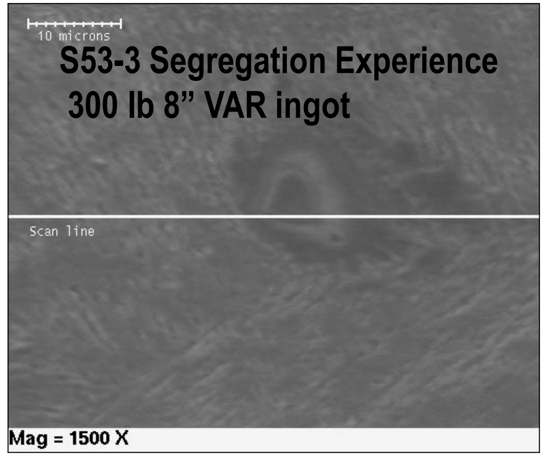
Results of 1000 runs (12 minutes on a Pentium IV 2.2GHz CPU)

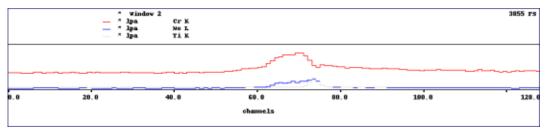


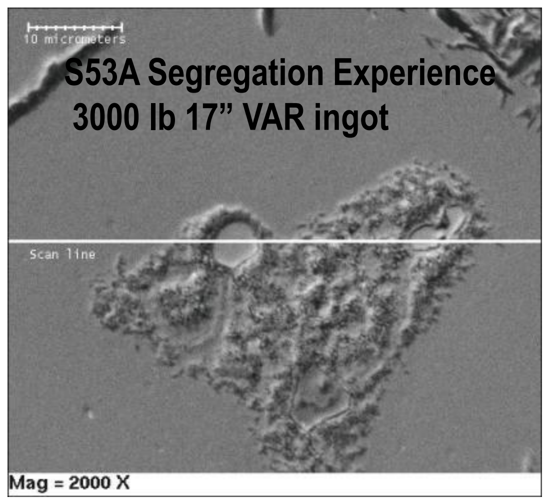
Ferrium S53 — Design For Scale

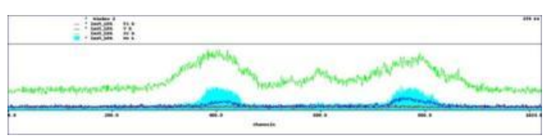


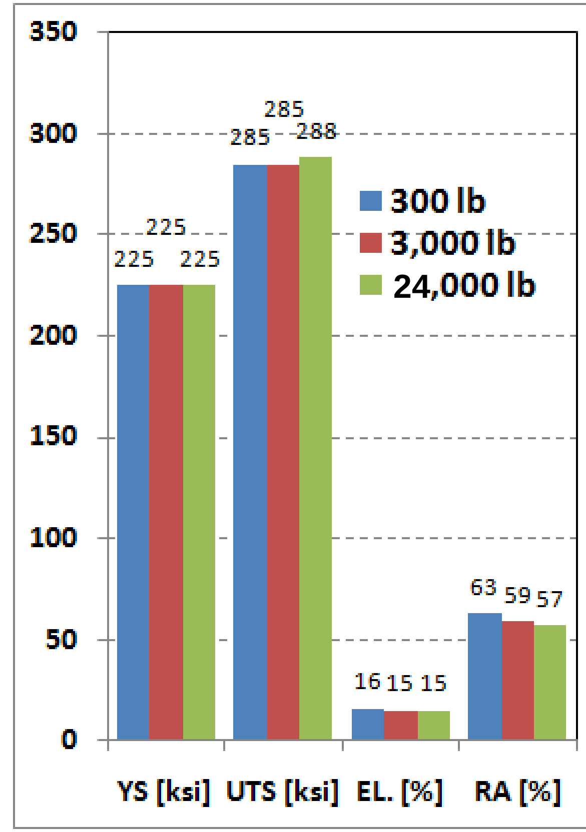




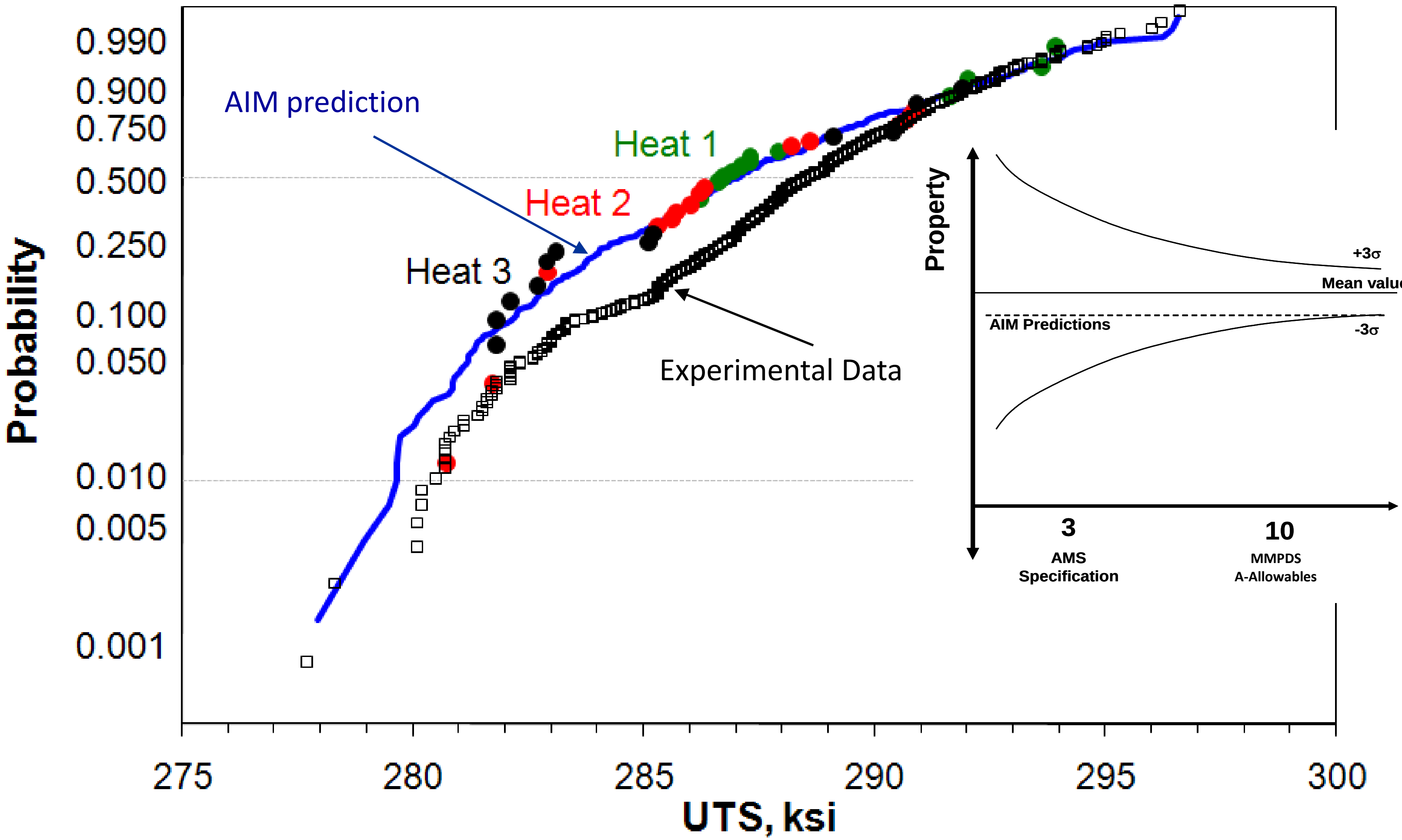




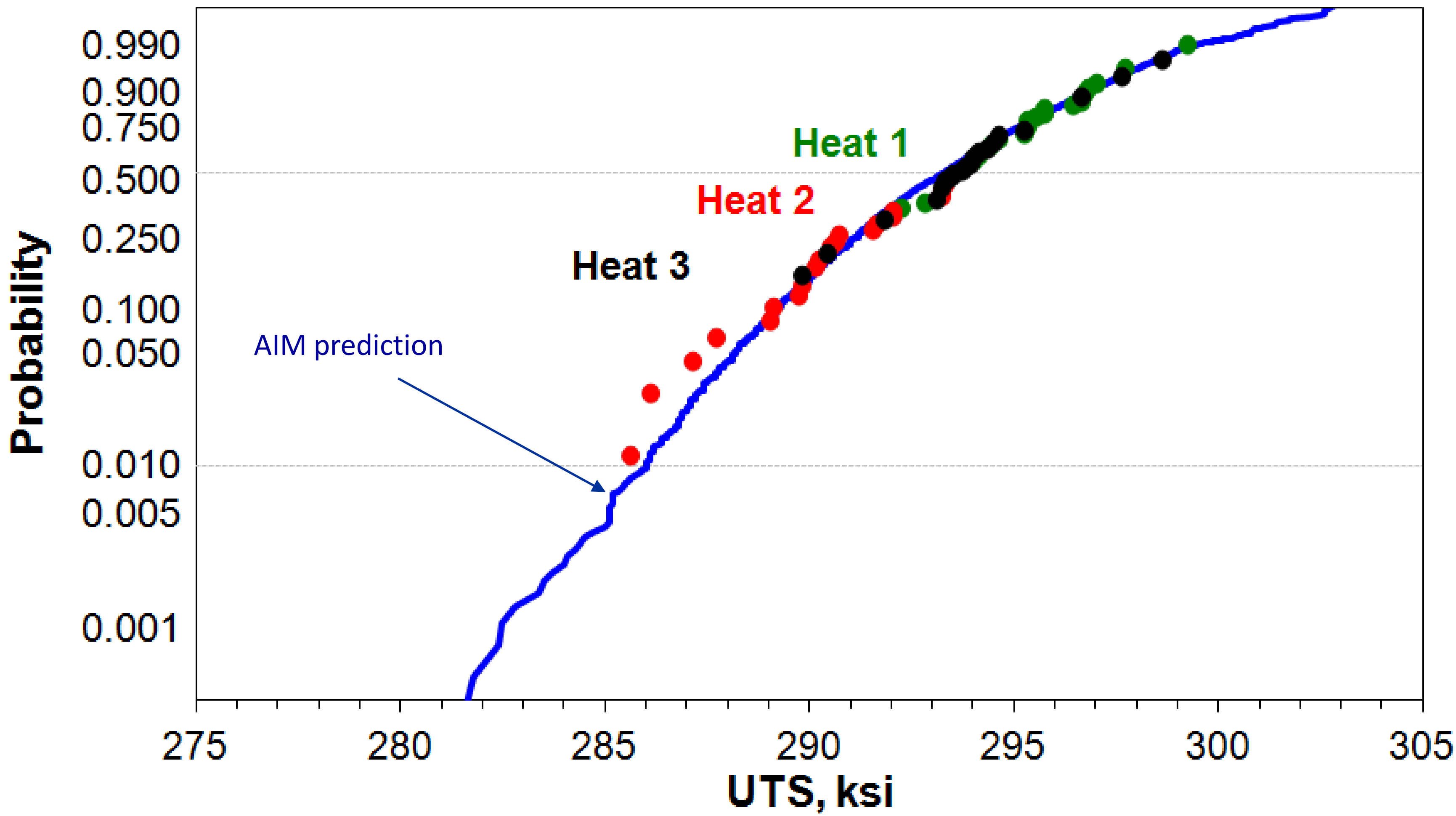




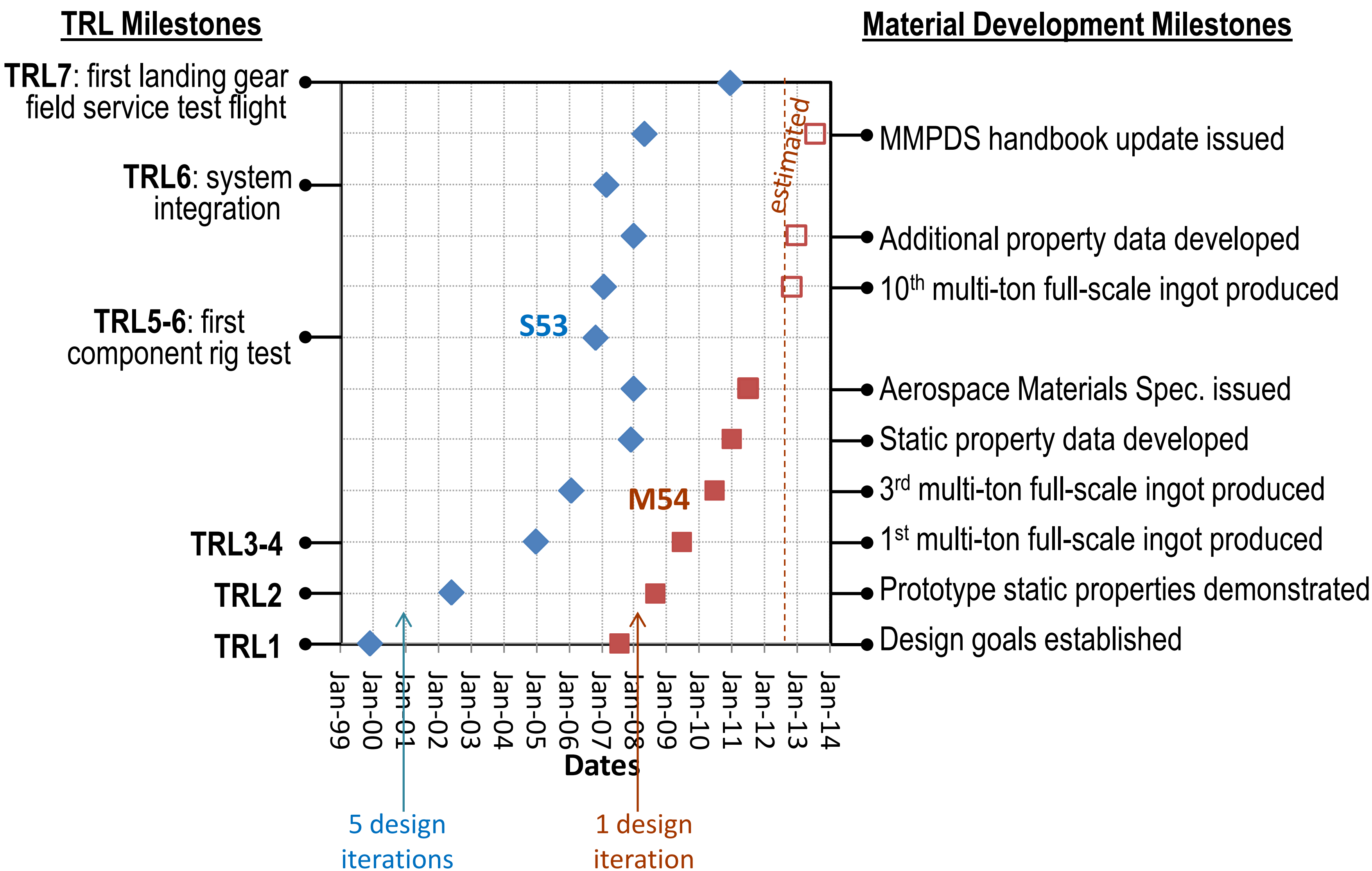
S53 AIM Analysis for UTS

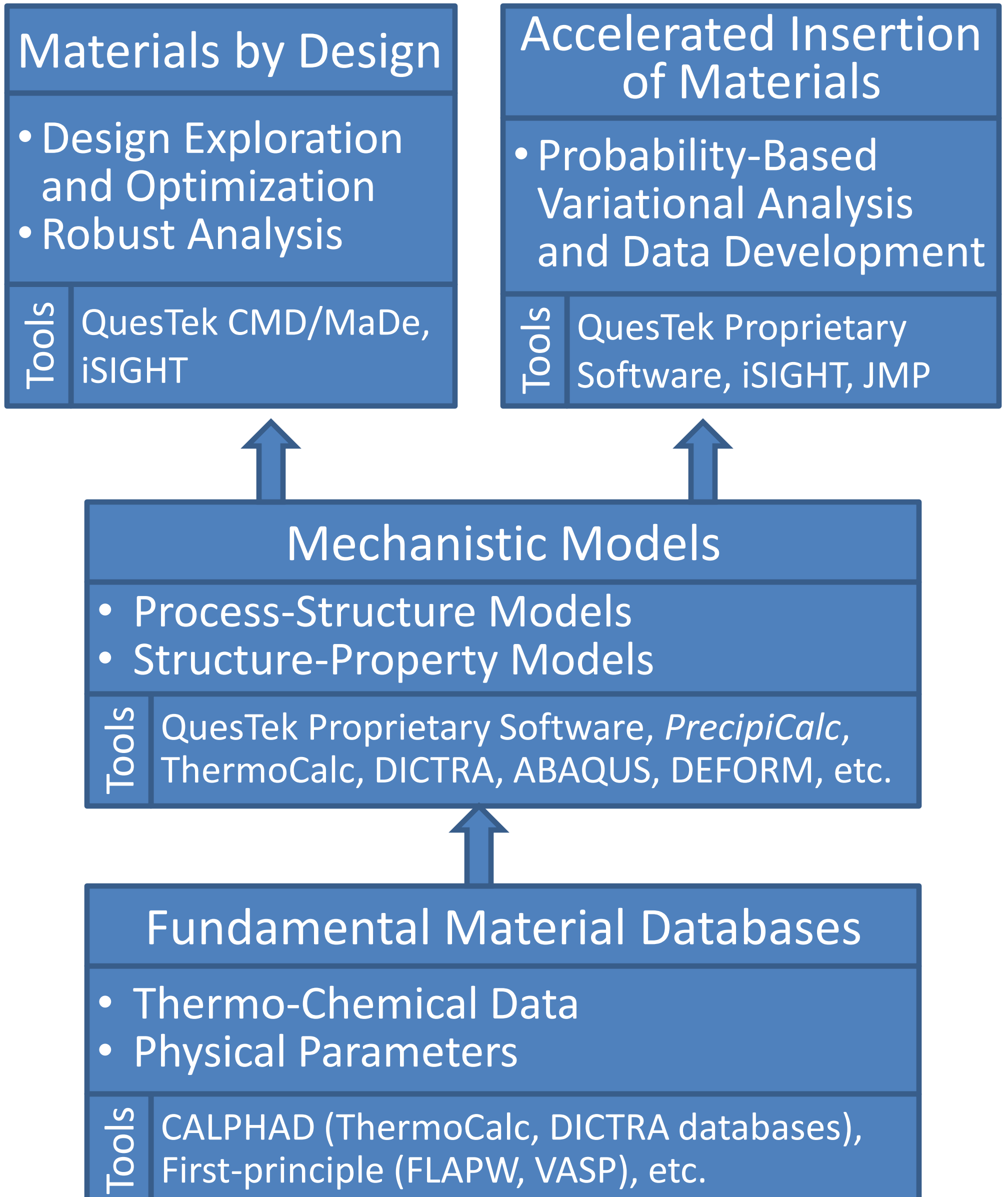


M54 AIM Analysis for UTS



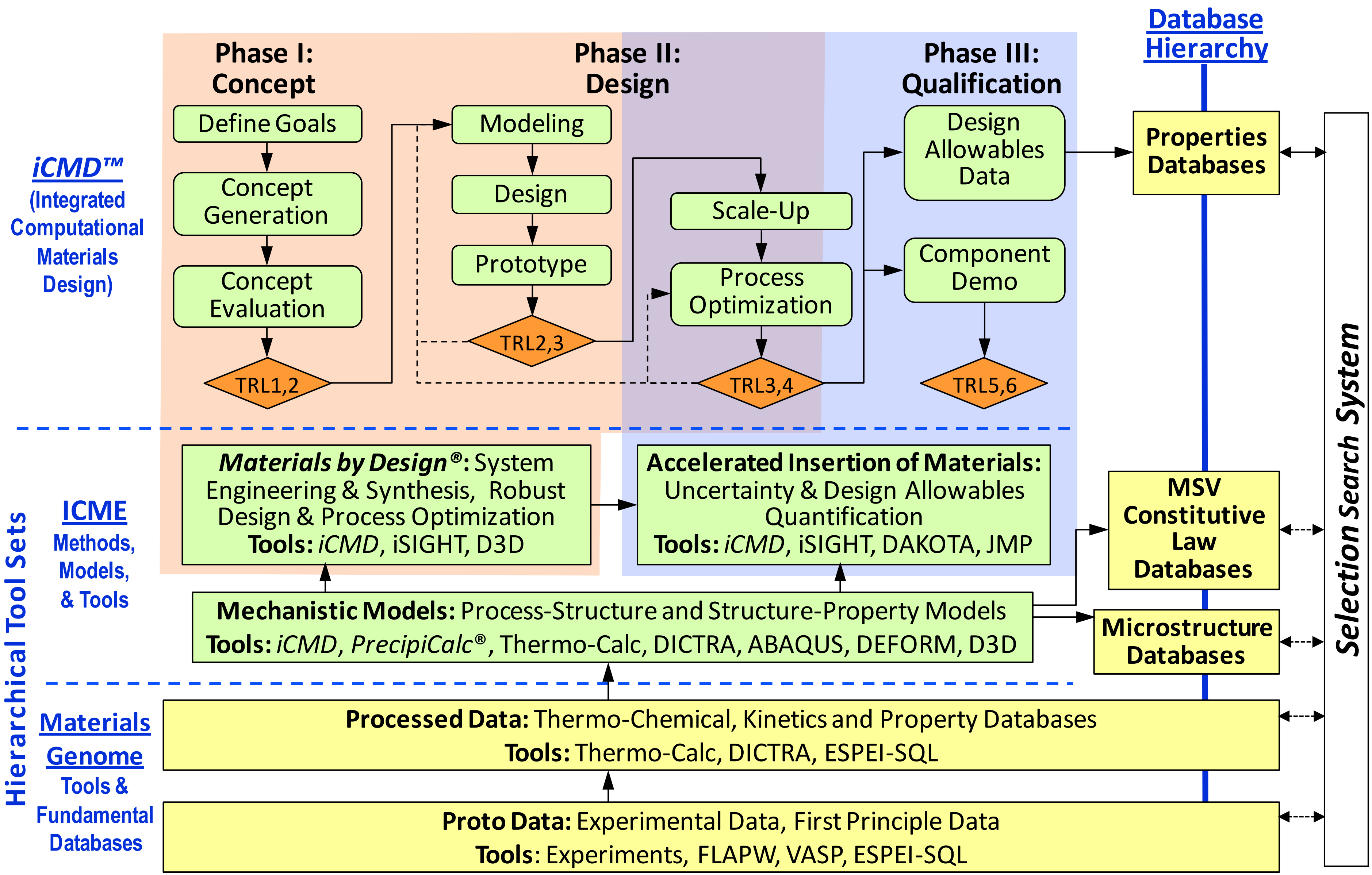
Computational Materials Qualification Acceleration

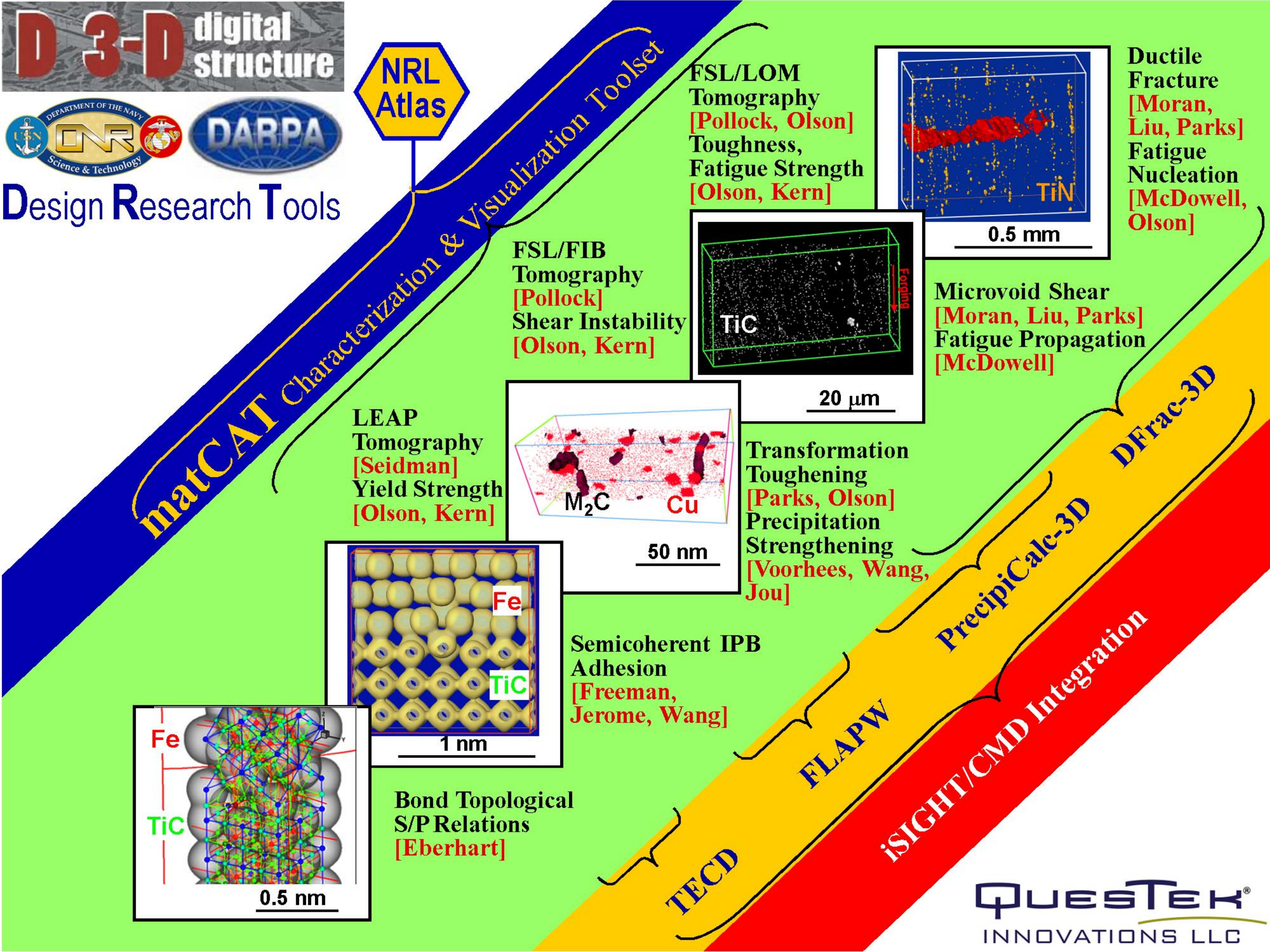



Materials by Design
• Design Exploration and Optimization
• Robust Analysis
Tools
QuesTek CMD/MaDe, iSIGHT
Accelerated Insertion of Materials
• Probability-Based Variational Analysis and Data Development
Tools
QuesTek Proprietary Software, iSIGHT, JMP
Mechanistic Models
• Process-Structure Models
• Structure-Property Models
Tools
QuesTek Proprietary Software, *PrecipiCalc*, ThermoCalc, DICTRA, ABAQUS, DEFORM, etc.
Fundamental Material Databases
• Thermo-Chemical Data
• Physical Parameters
Tools
CALPHAD (ThermoCalc, DICTRA databases), First-principle (FLAPW, VASP), etc.

ICME MS Program

	F	W	S
Required Core	MSc 401 Analytical & Statistical Thermodynamics PSED 510-1 (0.5) ICME Seminar	MSc 408 Phase Transformations in Materials MSc 458 Computational Materials	MSc 390 Materials Design PSED 510-2 (0.5) ICME Seminar
Recommended Electives	MSc 391 Process Design MSc/ESAM 495 Modeling of Soft Materials CEE327/ME 365 Introduction to FEM ME 341 Computational Methods for Engineering Design (or ME 441 Engineering Optimization for Product Design & Manufacturing)	MSc/ESAM 495 Introduction to Statistical Mechanics ME/CEE 426-1 Computational Mechanics I ME 366 Finite Elements for Design & Optimization	MSc 406 Mechanical Properties of Materials ME/CEE 426-2 Computational Mechanics II Phys 450 Advanced Computational Condensed Matter Physics


Database Hierarchy
Phase I: Concept
Phase II: Design
Phase III: Qualification
iCMD™ (Integrated Computational Materials Design)
Define Goals
Concept Generation
Concept Evaluation
TRL1,2
Modeling
Design
Prototype
TRL2,3
Scale-Up
Process Optimization
TRL3,4
Design Allowables Data
Component Demo
TRL5,6
Properties Databases
Hierarchical Tool Sets
ICME Methods, Models, & Tools
Materials by Design®: System Engineering & Synthesis, Robust Design & Process Optimization
Tools: iCMD, iSIGHT, D3D
Accelerated Insertion of Materials: Uncertainty & Design Allowables Quantification
Tools: iCMD, iSIGHT, DAKOTA, JMP
MSV Constitutive Law Databases
Mechanistic Models: Process-Structure and Structure-Property Models
Tools: iCMD, PrecipiCalc®, Thermo-Calc, DICTRA, ABAQUS, DEFORM, D3D
Microstructure Databases
Materials Genome Tools & Fundamental Databases
Processed Data: Thermo-Chemical, Kinetics and Property Databases
Tools: Thermo-Calc, DICTRA, ESPEI-SQL
Proto Data: Experimental Data, First Principle Data
Tools: Experiments, FLAPW, VASP, ESPEI-SQL
Selection Search System


D 3-D digital structure
DEPARTMENT OF THE NAVY
ONR
Science & Technology
DARPA
Design Research Tools
NRL Atlas
matCAT Characterization & Visualization Toolset
FSL/LOM Tomography
[Pollock, Olson]
Toughness, Fatigue Strength
[Olson, Kern]
TiN
0.5 mm
Ductile Fracture
[Moran, Liu, Parks]
Fatigue Nucleation
[McDowell, Olson]
FSL/FIB Tomography
[Pollock]
Shear Instability
[Olson, Kern]
TiC
Forging
20 μm
Microvoid Shear
[Moran, Liu, Parks]
Fatigue Propagation
[McDowell]
LEAP Tomography
[Seidman]
Yield Strength
[Olson, Kern]
M2C
Cu
50 nm
Transformation Toughening
[Parks, Olson]
Precipitation Strengthening
[Voorhees, Wang, Jou]
Fe
TiC
1 nm
Semicoherent IPB Adhesion
[Freeman, Jerome, Wang]
Fe
TiC
0.5 nm
Bond Topological S/P Relations
[Eberhart]
DFrac-3D
PrecipiCalc-3D
FLAPW
TECD
iSIGHT/CMD Integration
QuesTek® INNOVATIONS LLC

Technology Transfer

QuesTek Navy Alloy Designs

Marine Corps: M67854-05-C-0025

NAVAIR: N68335-05-C-0207 and N68335-07-C-0108

NAVAIR N68335-10-C-0174

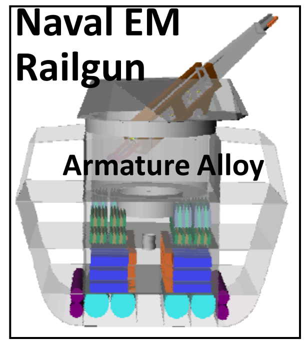
OSD N00014-09-M-0400

Marine Corps: M67854-10-C-6502

NAVAIR: N68335-07-C-0302 and N68335-08-C-0288

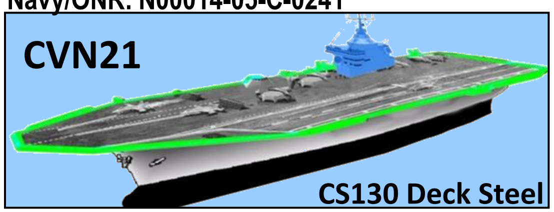
ONR: N00014-07-M-0445 STTR-I

ONR: N00014-09-M-0220



NAVAIR: N68335-07-C-0428

Navy/ONR: N00014-05-C-0241



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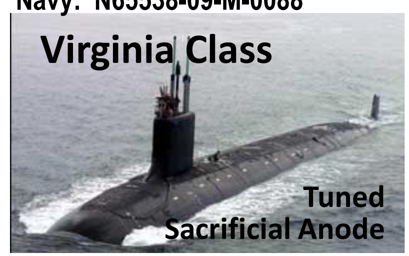


ONR: N00014-08-M-0309

ONR: N00014-05-M-0250
NAVAIR: N68335-06-C-0339

NAVAIR: N68335-09-C-0215

NAVAIR N68335-10-C-0229

MSc390 Materials Design

Spring 2012
Design Projects

I. **Civil Shield (EDC)**
Client: ONR, DHS, Trinity R
Advisor: Dr. Zack Feinberg
Team: Ma, Maethasith, Richardson, Schwenker, Zhao

II. **Earthquake Steel**
Client: ArcelorMittal
Advisor: George Fraley
Team: Cool, Gross, Rawlings, Tran

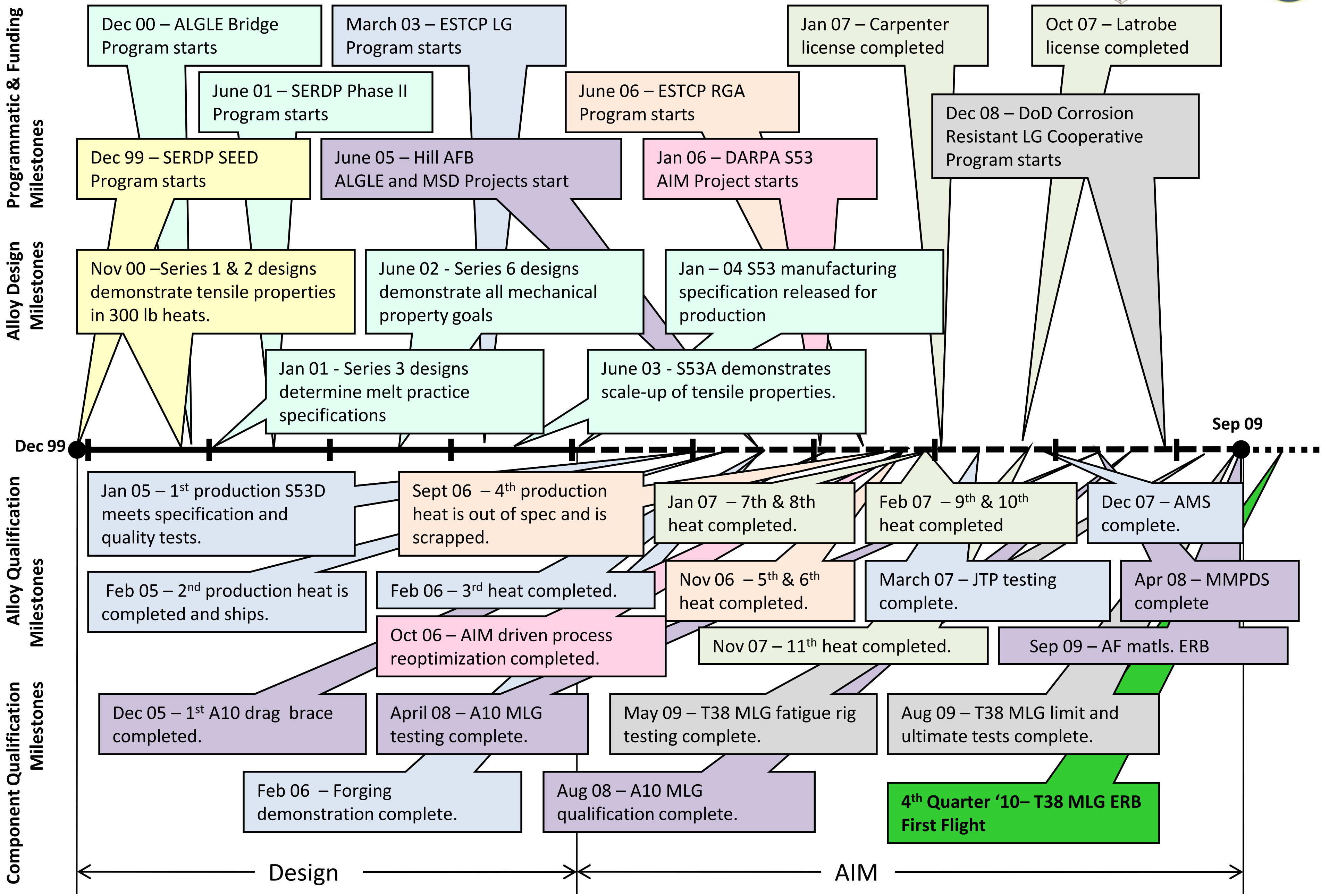
III. **FSW Joinable Aluminum**
Client: Boeing, Ford
Advisor: Ricardo Komai
Team: Brodnik, McGinnis, Pai, Ricks

IV. **HP Magnesium**
Client: ARO, GM, DOE
Advisor: Dr. Dennis Zhang
Team: Han, Na, Park

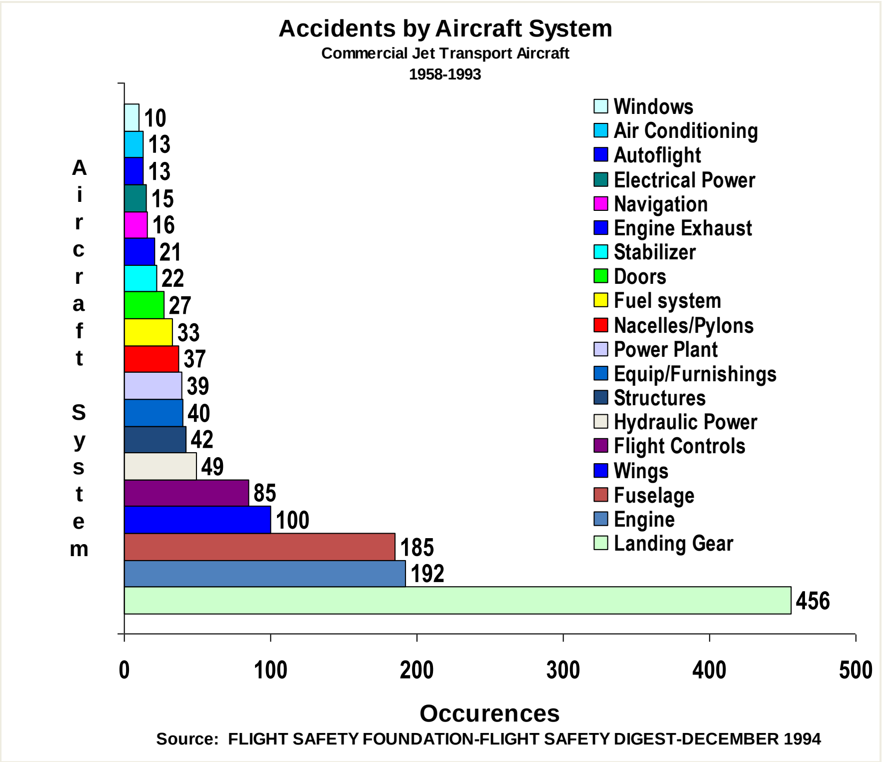
V. **TRIP Titanium**
Client: ONR
Advisor: Jiayi Yan
Team: Savoie, Wengrenovich

VI. **HP Shape Memory Alloy (EDC)**
Client: Medtronic, GM
Advisor: Dana Frankel
Team: Jin, Kadleck, Poupard, Yoo

S53 Transition Milestones



UHS Stainless Steels for Landing Gear



SCC failure

HE failure

Issues:

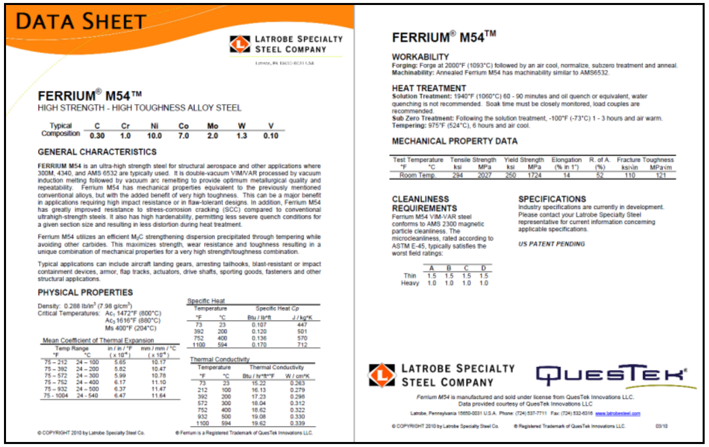
- *Over $200M spent in LG per year*
- *80% corrosion related SCC failures*
- *Cad plating used to protect current steel*
- *Known carcinogen (AF 2000 lb/yr)*

Stainless Benefits:

- *Dramatic reduction in LG cost (60%= $120M per year)*
- *Significant reduction in SCC failures*
- *Cadmium plating not required*
- *General corrosion mitigated*
- *80% of Steel Condemnations Avoided*

M54: NAVAIR SBIR program goals for LG steels

- Enhanced landing gear life
- Navy replacement for AMS 6532 (Aermet®100)
  - Equivalent-to-better properties
    - Tensile (including ductility)
    - Fracture toughness
    - SCC resistance
  - Significantly lower cost



DATA SHEET

LATROBE SPECIALTY STEEL COMPANY

FERRIUM® M54™

HIGH STRENGTH - HIGH TOUGHNESS ALLOY STEEL

Typical Composition	C	Cr	Ni	Co	Mo	W	V
	0.30	1.0	10.0	7.0	2.0	1.3	0.10

GENERAL CHARACTERISTICS

FERRIUM M54 is an ultra-high strength steel for structural aerospace and other applications where 300M, 4340, and AMS 6532 are typically used. It is double-vacuum VIM/VAR processed by vacuum induction melting followed by vacuum arc remelting to provide optimum metallurgical quality and repeatability. Ferrium M54 has mechanical properties equivalent to the previously mentioned conventional alloys, but with the added benefit of very high toughness. This can be a major benefit in applications requiring high impact resistance or in flaw-tolerant designs. In addition, Ferrium M54 has greatly improved resistance to stress-corrosion cracking (SCC) compared to conventional ultrahigh-strength steels. It also has high hardenability, permitting less severe quench conditions for a given section size and resulting in less distortion during heat treatment.

Ferrium M54 utilizes an efficient M_2C strengthening dispersion precipitated through tempering while avoiding other carbides. This maximizes strength, wear resistance and toughness resulting in a unique combination of mechanical properties for a very high strength/toughness combination.

Typical applications can include aircraft landing gears, arresting tailhooks, blast-resistant or impact containment devices, armor, flap tracks, actuators, drive shafts, sporting goods, fasteners and other structural applications.

PHYSICAL PROPERTIES

Density: 0.288 lb/in³ (7.98 g/cm³)
Critical Temperatures: Ac_1 1472°F (800°C), Ac_3 1616°F (880°C), Ms 400°F (204°C)

Mean Coefficient of Thermal Expansion

Temp Range °F	Temp Range °C	in / in / °F (x 10⁻⁶)	mm / mm / °C (x 10⁻⁶)
75 – 212	24 – 100	5.65	10.17
75 – 392	24 – 200	5.82	10.47
75 – 572	24 – 300	5.99	10.78
75 – 752	24 – 400	6.17	11.10
75 – 932	24 – 500	6.37	11.47
75 - 1004	24 - 540	6.47	11.64

Specific Heat

Temperature °F	Temperature °C	Specific Heat Cp Btu / lb*ft	Specific Heat Cp J / kg*K
73	23	0.107	447
392	200	0.120	501
752	400	0.136	570
1100	594	0.170	712

Thermal Conductivity

Temperature °F	Temperature °C	Thermal Conductivity Btu / hr*ft*°F	Thermal Conductivity W / cm*K
73	23	15.22	0.263
212	100	16.13	0.279
392	200	17.23	0.298
572	300	18.04	0.312
752	400	18.62	0.322
932	500	19.08	0.330
1100	594	19.62	0.339

FERRIUM® M54™

WORKABILITY

Forging: Forge at 2000°F (1093°C) followed by an air cool, normalize, subzero treatment and anneal.
Machinability: Annealed Ferrium M54 has machinability similar to AMS6532.

HEAT TREATMENT

Solution Treatment: 1940°F (1060°C) 60 - 90 minutes and oil quench or equivalent, water quenching is not recommended. Soak time must be closely monitored, load couples are recommended.
Sub Zero Treatment: Following the solution treatment, -100°F (-73°C) 1 - 3 hours and air warm.
Tempering: 975°F (524°C), 6 hours and air cool.

MECHANICAL PROPERTY DATA

Test Temperature °F	Test Temperature °C	Tensile Strength ksi	Tensile Strength MPa	Yield Strength ksi	Yield Strength MPa	Elongation (% in 1")	R. of A. (%)	Fracture Toughness ksi√in	Fracture Toughness MPa√m
Room Temp.		294	2027	250	1724	14	52	110	121

CLEANLINESS REQUIREMENTS

Ferrium M54 VIM-VAR steel conforms to AMS 2300 magnetic particle cleanliness. The microcleanliness, rated according to ASTM E-45, typically satisfies the worst field ratings:

	A	B	C	D
Thin	1.5	1.5	1.5	1.5
Heavy	1.0	1.0	1.0	1.0

SPECIFICATIONS

Industry specifications are currently in development. Please contact your Latrobe Specialty Steel representative for current information concerning applicable specifications.

US PATENT PENDING

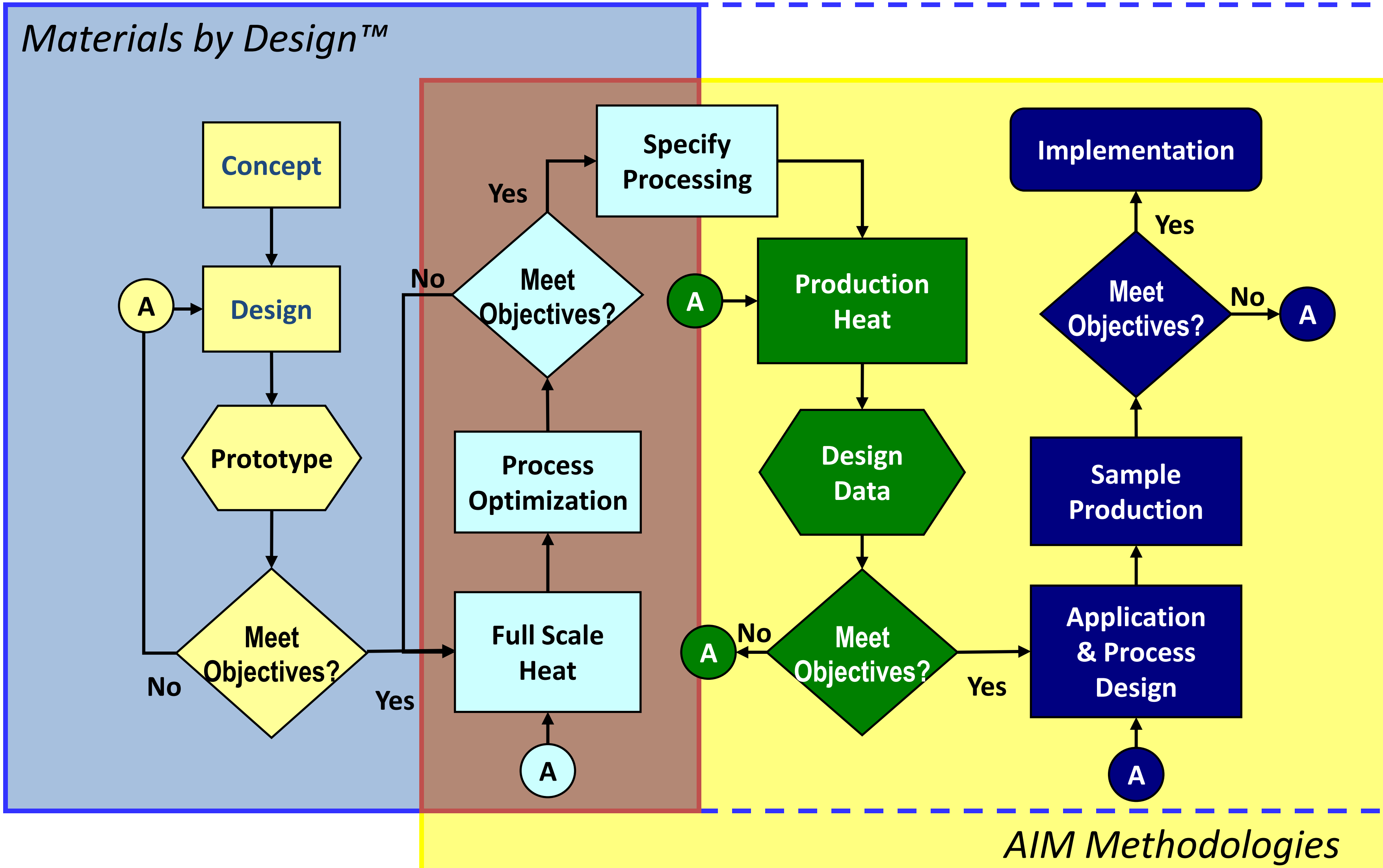
LATROBE SPECIALTY STEEL COMPANY QUESTEK®

Ferrium M54 is manufactured and sold under license from QuesTek Innovations LLC.
Data provided courtesy of QuesTek Innovations LLC

Latrobe, Pennsylvania 15650-0031 U.S.A. Phone: (724) 537-7711 Fax: (724) 532-6316 www.latrobesteel.com

AMS 6516

Materials Development Cycle



Design Integration