materials design

Materials Design
2024 UGM Webinar Series

Genomic Materials Design:
Enabling Concurrency

Professor Greg B. Olson
MIT and QuesTek Innovations LLC

CHiMaD

QuesTek INNOVATIONS LLC

October 22, 2024

Materials Design UGM


UGM 2024
The Materials Design annual user event will be online for 2024.
Tuesdays and Thursdays
October 15 – November 7
Plenary Speakers:
Professor Sir Richard Catlow - University College London, England
Professor Georg Kresse, Dr. Martijn Marsman,
and Dr. Manuel Engel - The University of Vienna, Austria
Professor Greg Olson - Massachusetts Institute of Technology, USA
Dr. Céline Chizallet - IFP Energies Nouvelles, France
https://ugm.materialsdesign.com/

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Genomic Materials Design:
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October 22, 2024

Materials Design UGM Presenter

Professor Greg Olson

Thermo-Calc Professor of the Practice

Department of Materials Science and Engineering

Massachusetts Institute of Technology and

Co-founder

QuesTek Innovations LLC, USA

Webinar Speakers

Katherine Hollingsworth
khollingsworth@materialsdesign.com

Dr. Clive Freeman
cfreeman@materialsdesign.com

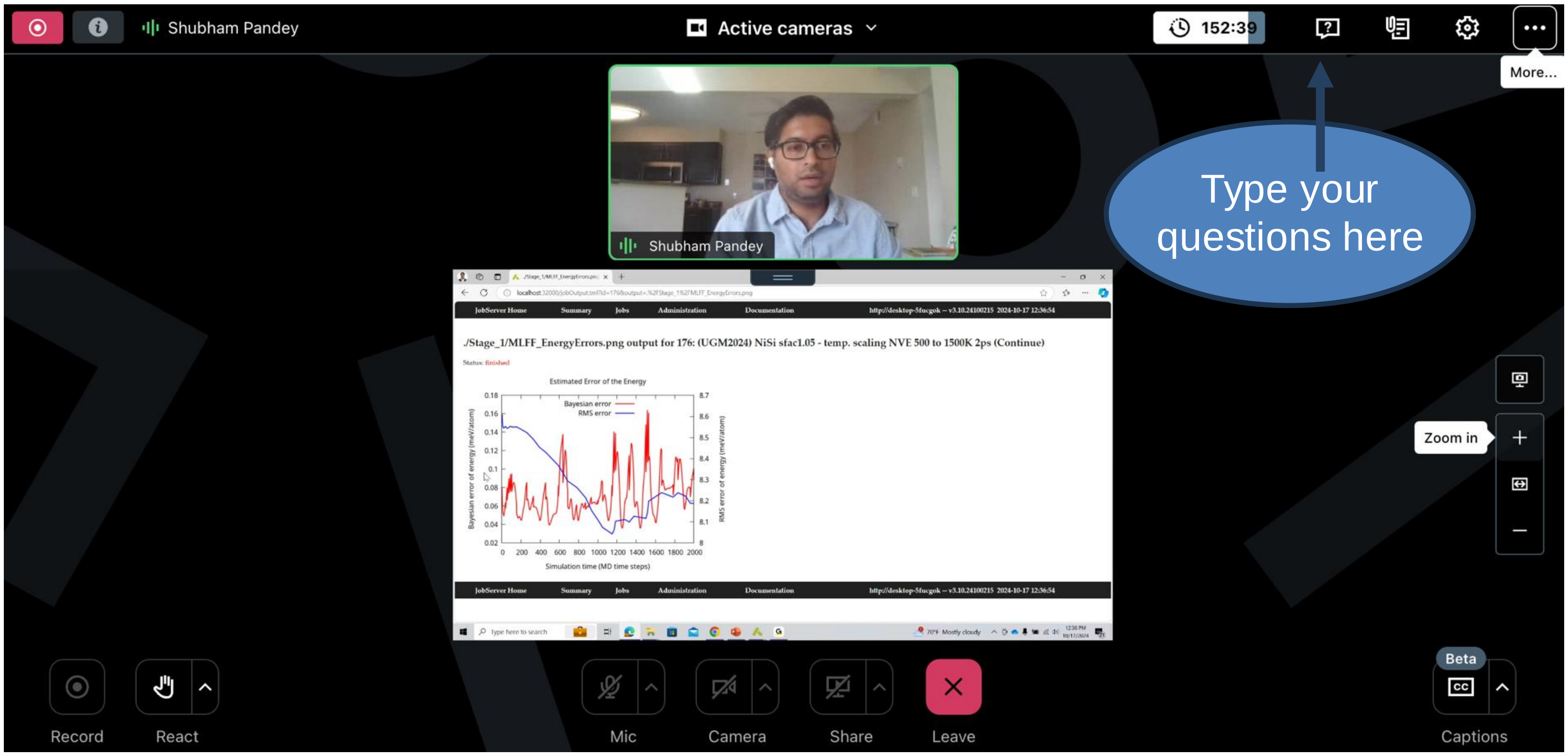
Materials Design UGM Webinar Series

- Share the plenary sessions with your colleagues!
  - Registration details

    https://www.ugm.materialsdesign.com
- We will be recording this session
  - Upcoming sessions are posted on the UGM site
  - Watch any of our earlier webinars anytime www.materialsdesign.com/webinars
- Brief survey
  - Take a 2 minutes brief survey at the end of the webinar
- Audio issues
  - Log out and log back in again
  - Check your audio output
  - Google Chrome (most recent 2 versions) Mozilla Firefox (most recent 2 versions) Apple Safari (most recent 2 versions) Microsoft Edge (most recent 2 versions)

materials design

Please Ask Questions!



Genomic Materials Design: Enabling Concurrency

G.B. Olson

MIT

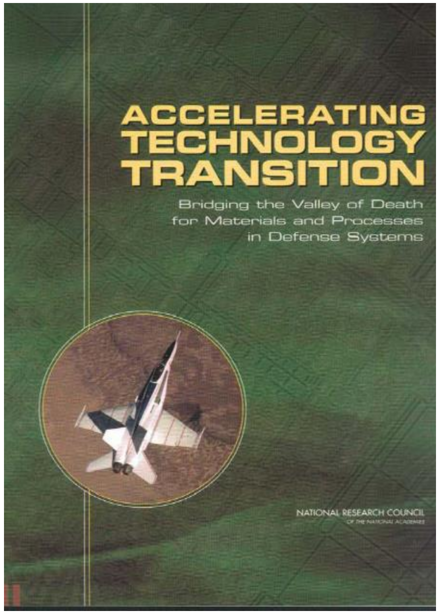
& QuesTek Innovations LLC

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.

NRC 2004 “Accelerating Technology Transition”
-Small Business ICME Supply Chain

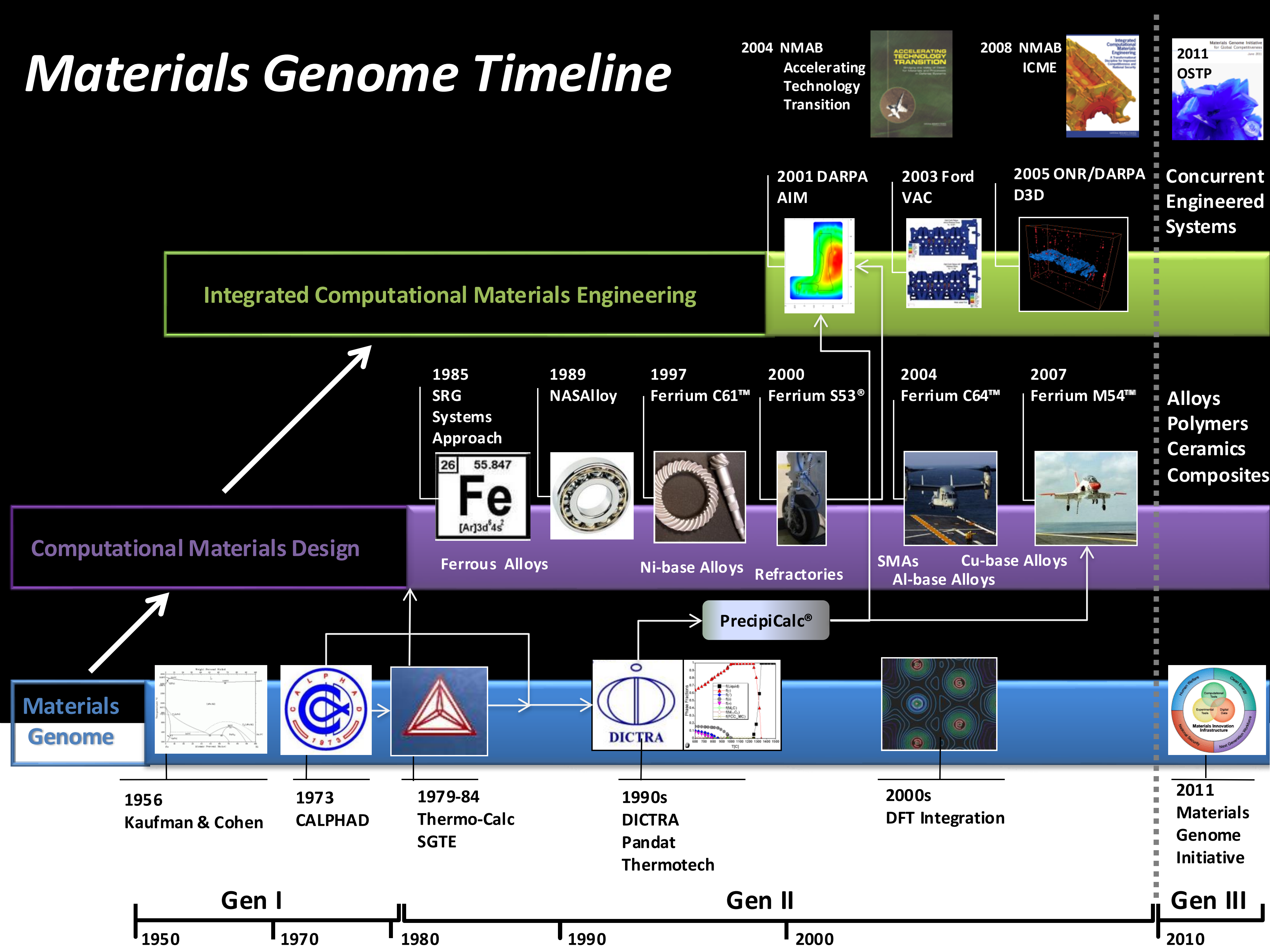
TABLE 3.1 Some Computational Materials Engineering Tools

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

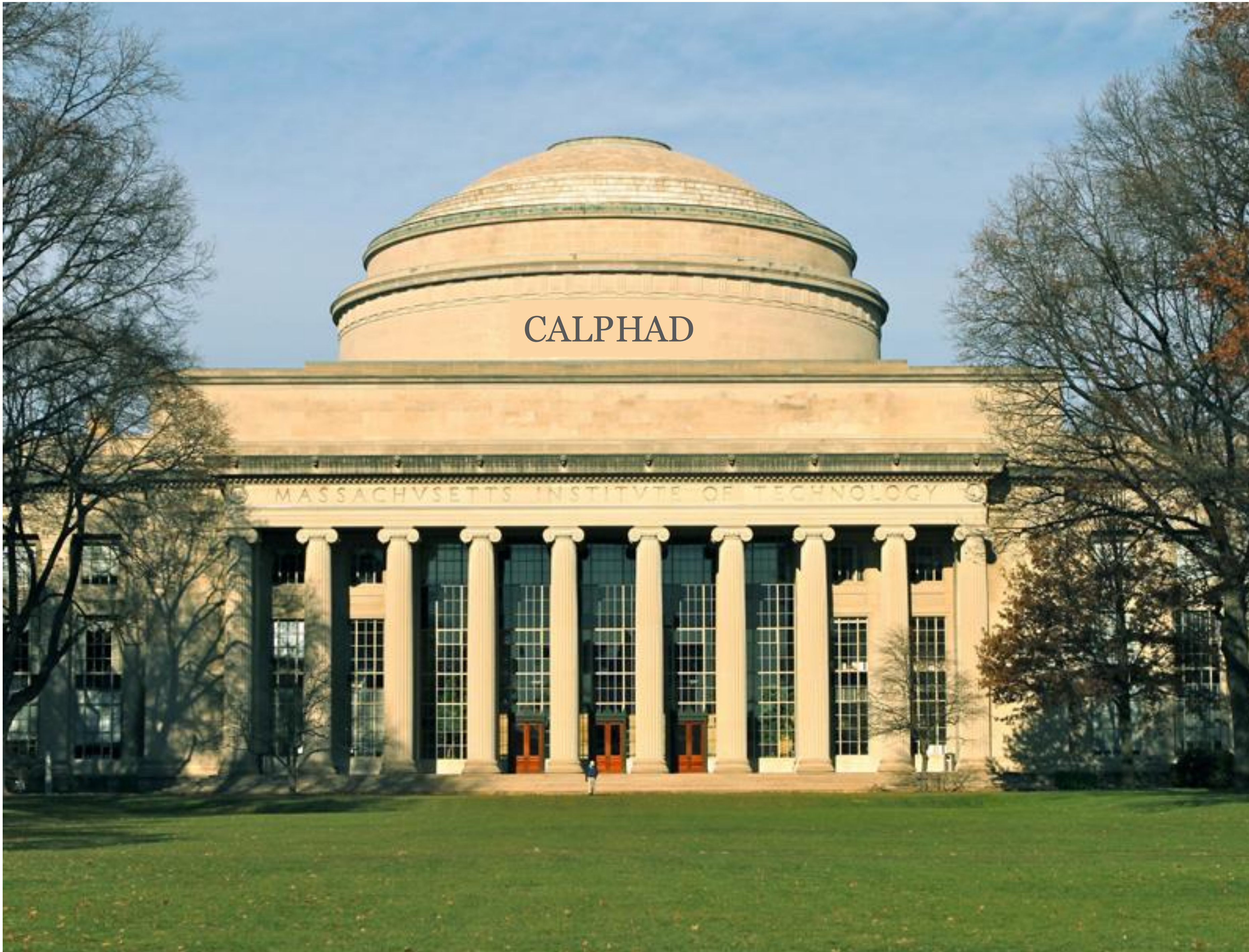
First Flight: QuesTek *Ferrium* S53®
T-38 main landing gear piston
December 17, 2010

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

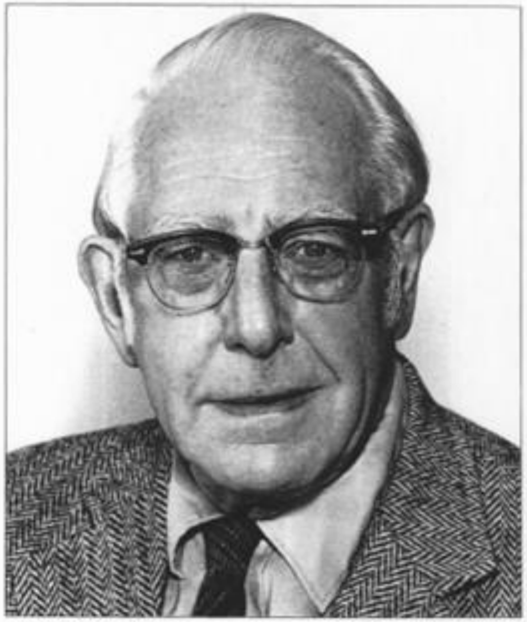
QuesTek® INNOVATIONS LLC



Materials Genome Timeline
2004 NMAB Accelerating Technology Transition
2008 NMAB ICME
2011 OSTP
2001 DARPA AIM
2003 Ford VAC
2005 ONR/DARPA D3D
Concurrent Engineered Systems
Integrated Computational Materials Engineering
1985 SRG Systems Approach
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
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


CALPHAD
MASSACHVSETTS INSTITVTE OF TECHNOLOGY

STRUCTURE- C.S. Smith



Interactive Hierarchy

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

} duality of description

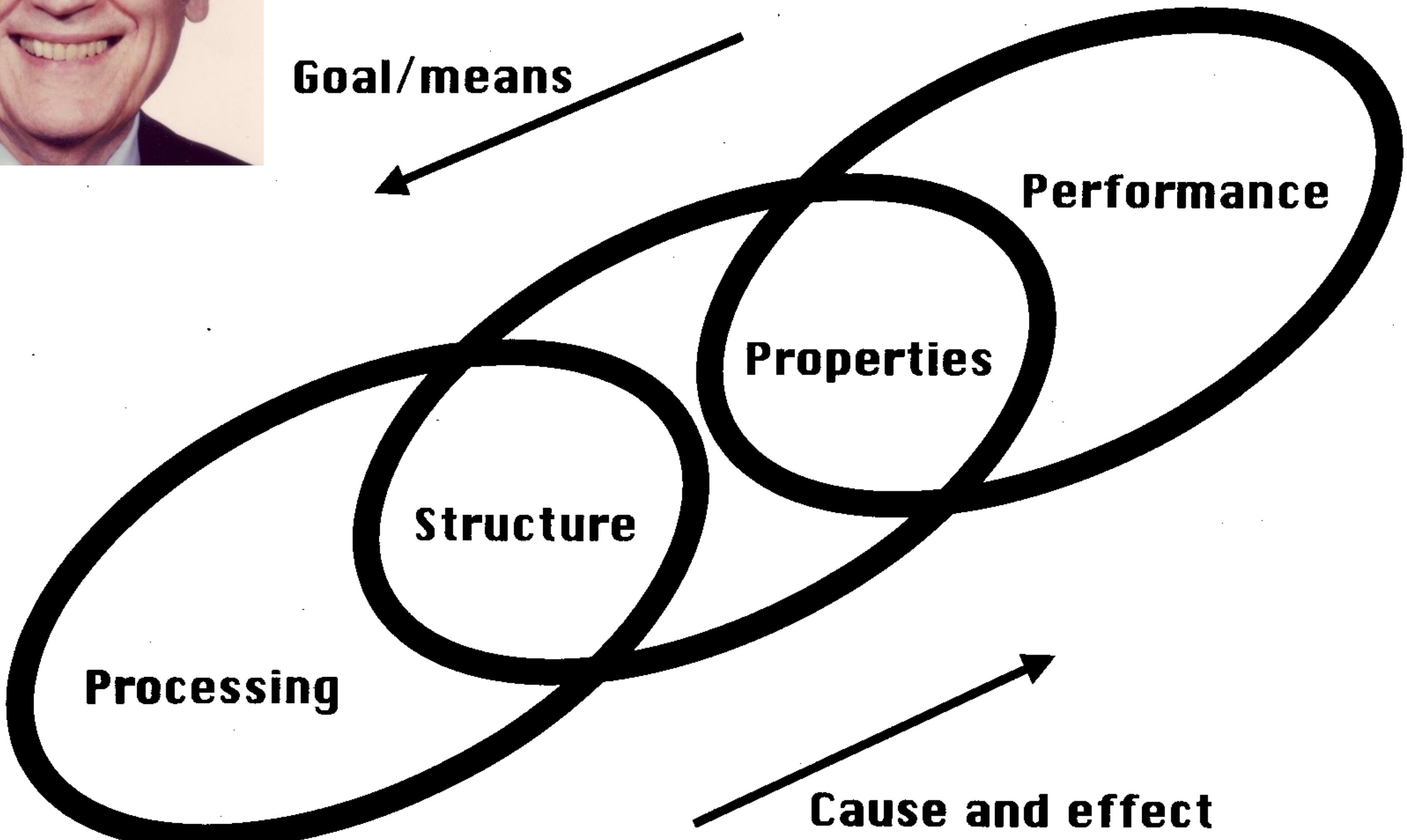
Real Complexity vs. Idealized Simplicity

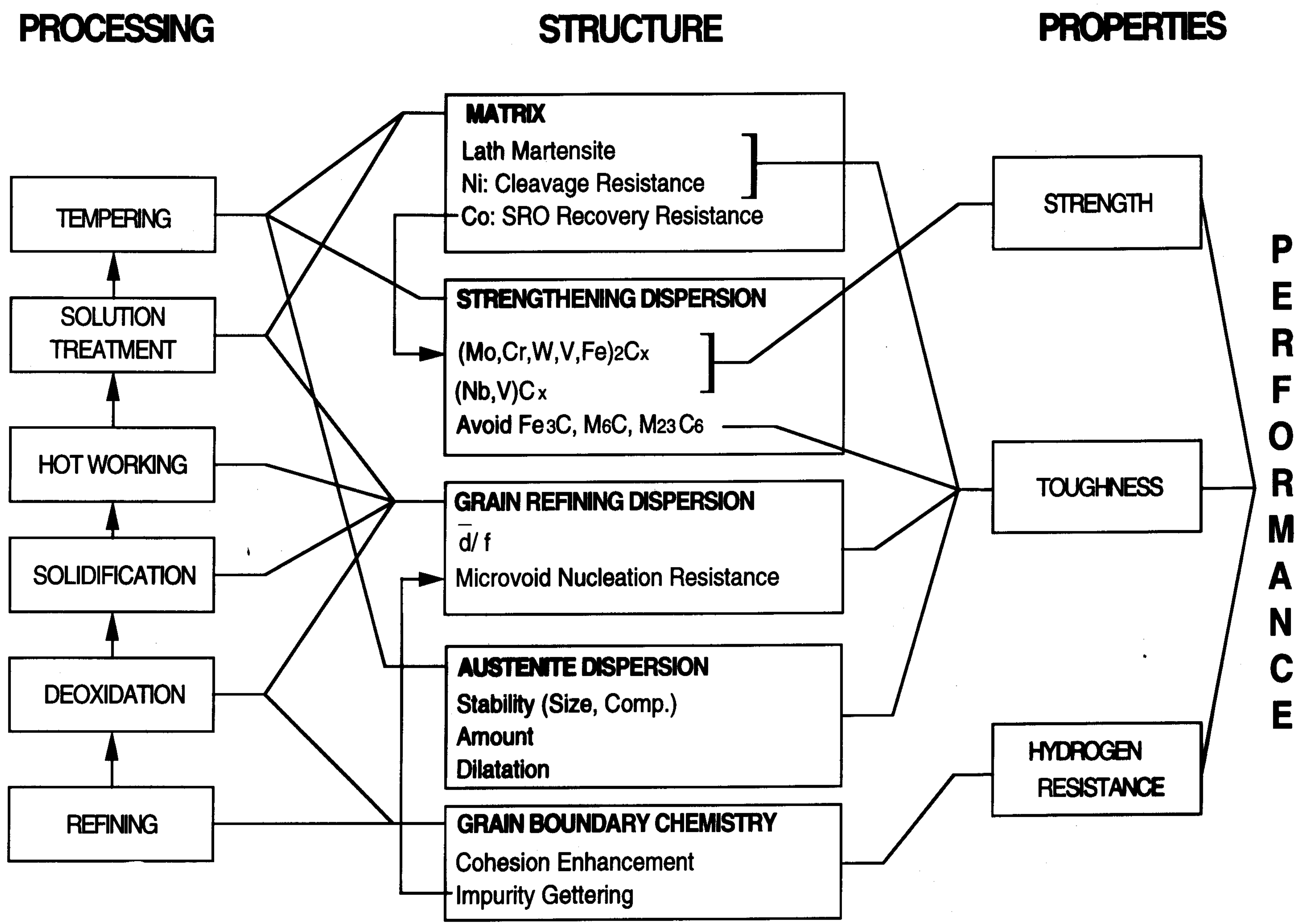
- -Cartesian Corpuscular Philosophy
- -Atom/Continuum

Dynamics

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

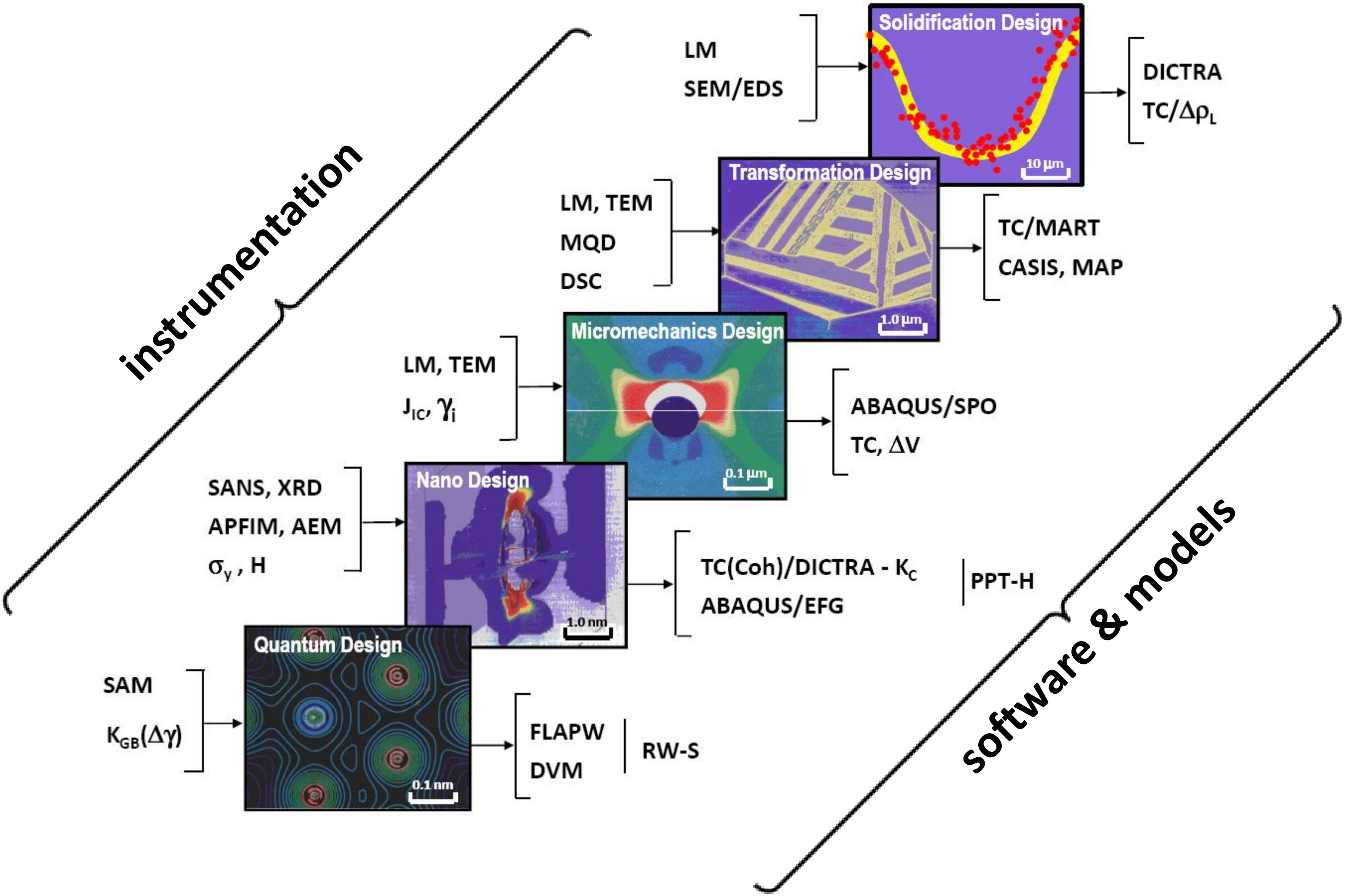
Cohen's Reciprocity



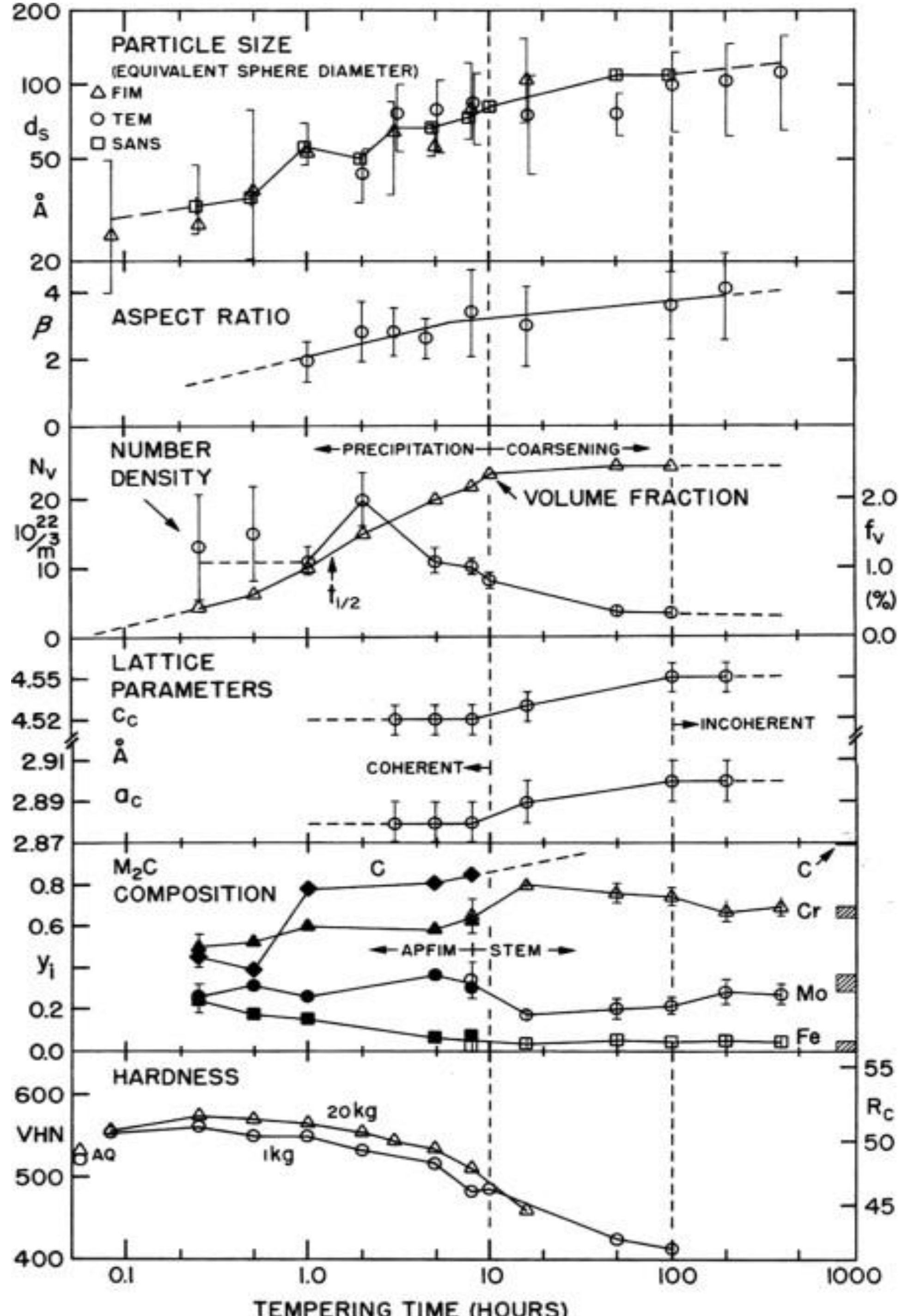


PROCESSING
STRUCTURE
PROPERTIES
TEMPERING
SOLUTION TREATMENT
HOT WORKING
SOLIDIFICATION
DEOXIDATION
REFINING
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
STRENGTHENING DISPERSION
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
GRAIN REFINING DISPERSION
d/ f
Microvoid Nucleation 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 strengthening: AF1410 (510C)



Thermodynamics of Strength

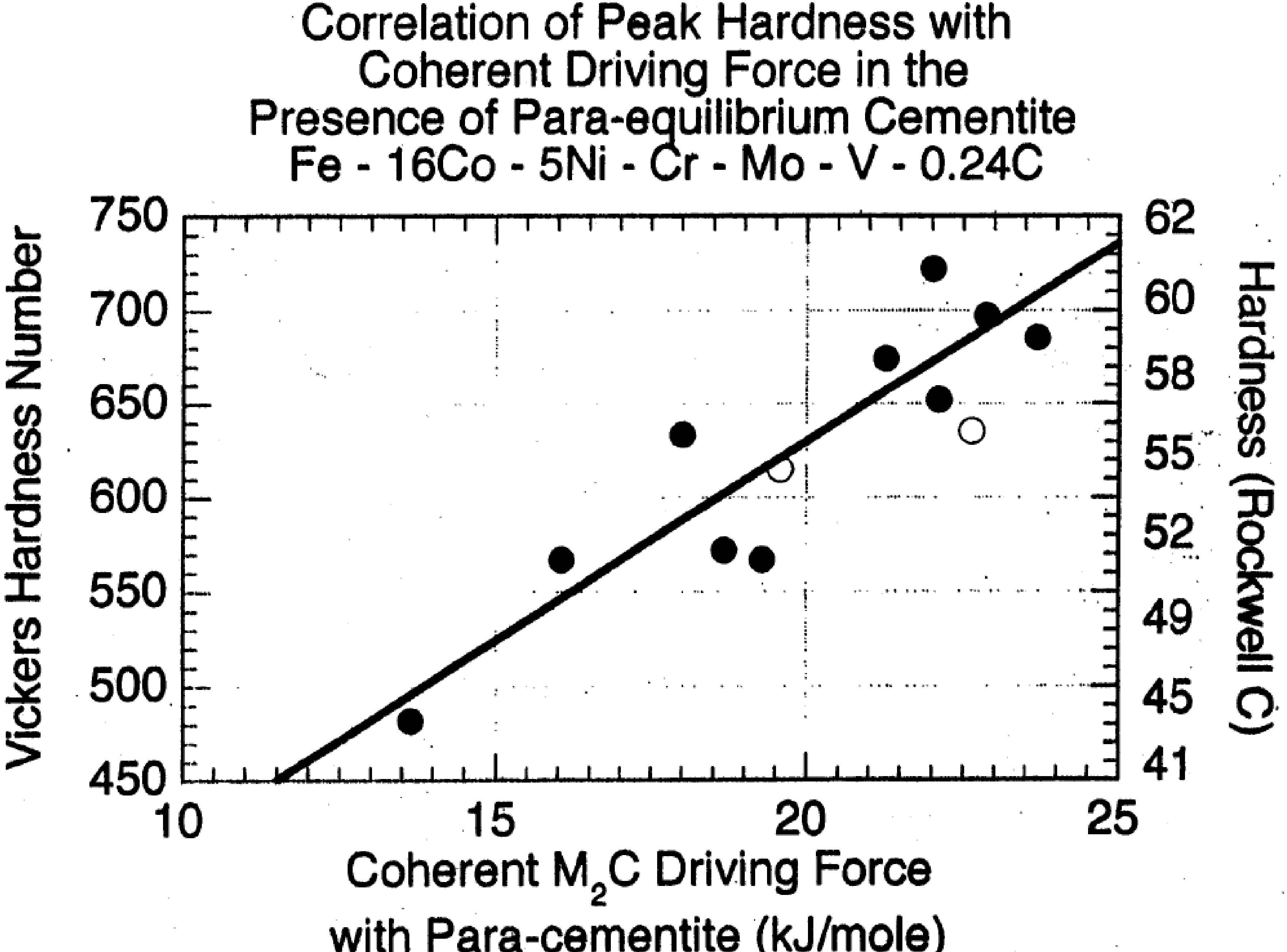
$$\Delta\tau_{Or} = K_1 \frac{\mu b}{\lambda}$$

$$\lambda \propto \frac{d}{f^{1/2}}$$

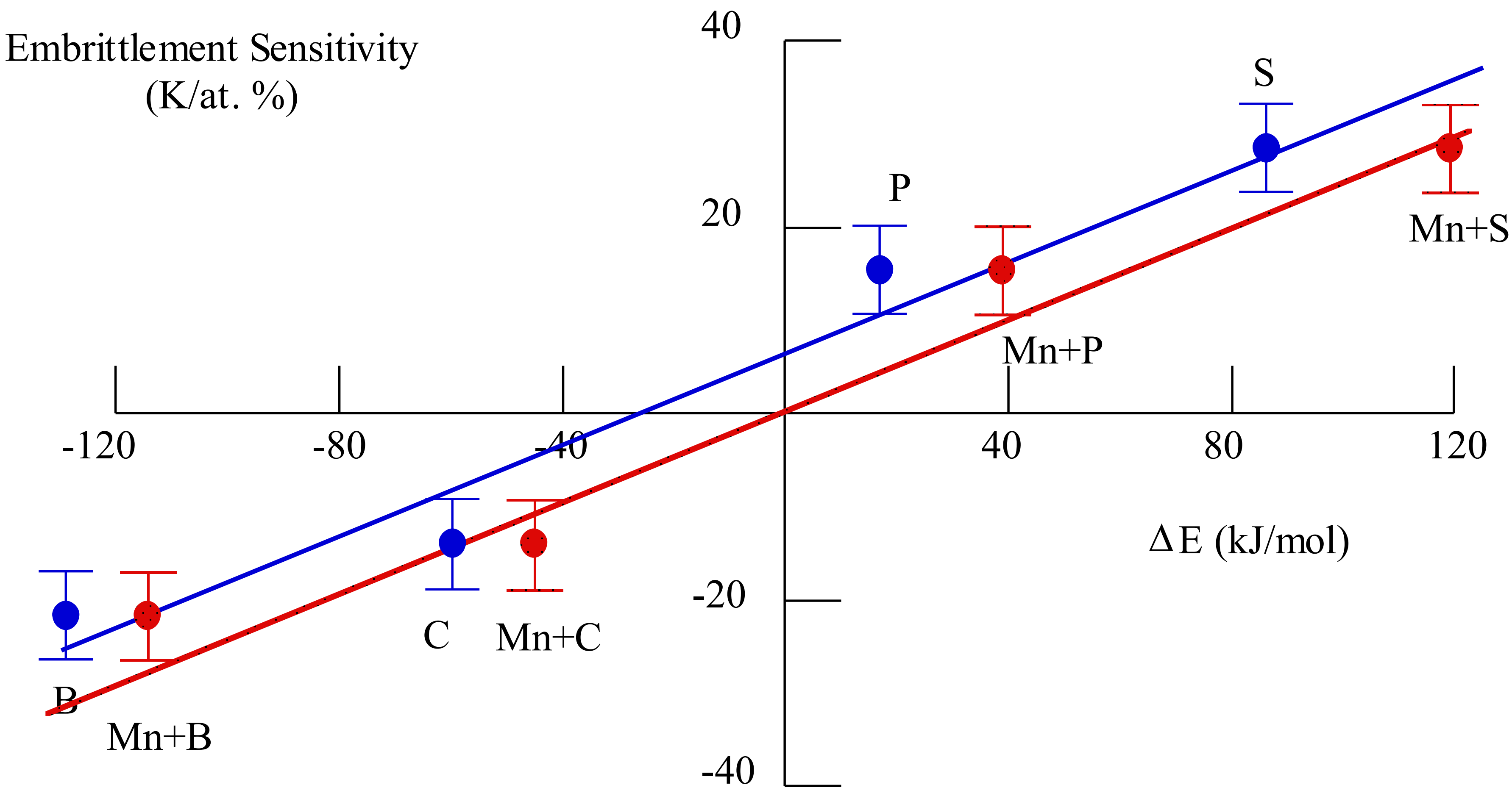
$$\Delta\tau_{Or} = K_2 \frac{f^{1/2}}{d}$$

$$d \propto |\Delta G|^{-1}$$

$$\Delta\tau_{Or} = K_3 \, |\Delta G| \, f^{1/2}$$

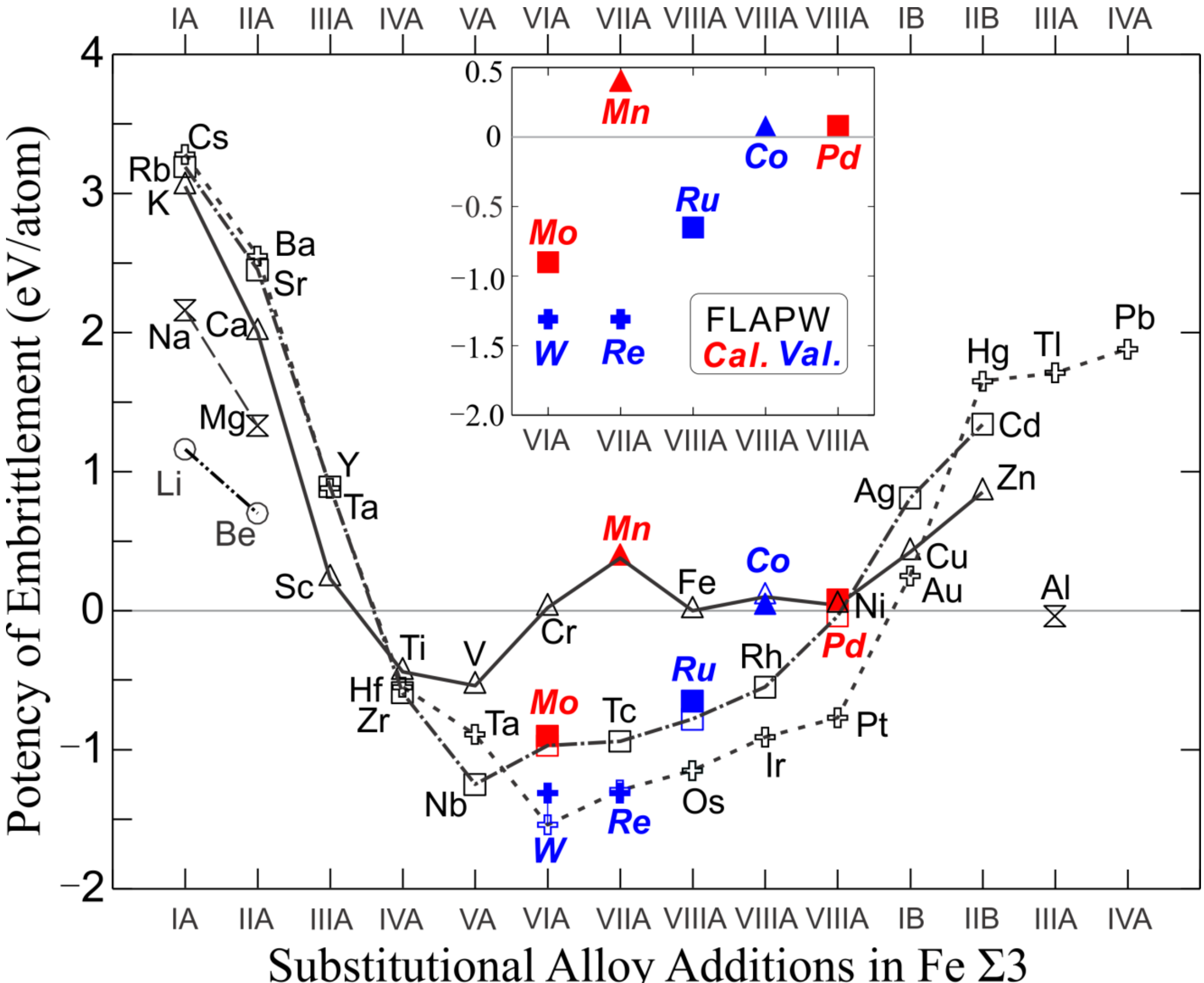

Correlation of Peak Hardness with
Coherent Driving Force in the
Presence of Para-equilibrium Cementite
Fe - 16Co - 5Ni - Cr - Mo - V - 0.24C
Vickers Hardness Number
750
700
650
600
550
500
450
Hardness (Rockwell C)
62
60
58
55
52
49
45
41
10
15
20
25
Coherent M_2C Driving Force
with Para-cementite (kJ/mole)

Grain Boundary Embrittlement



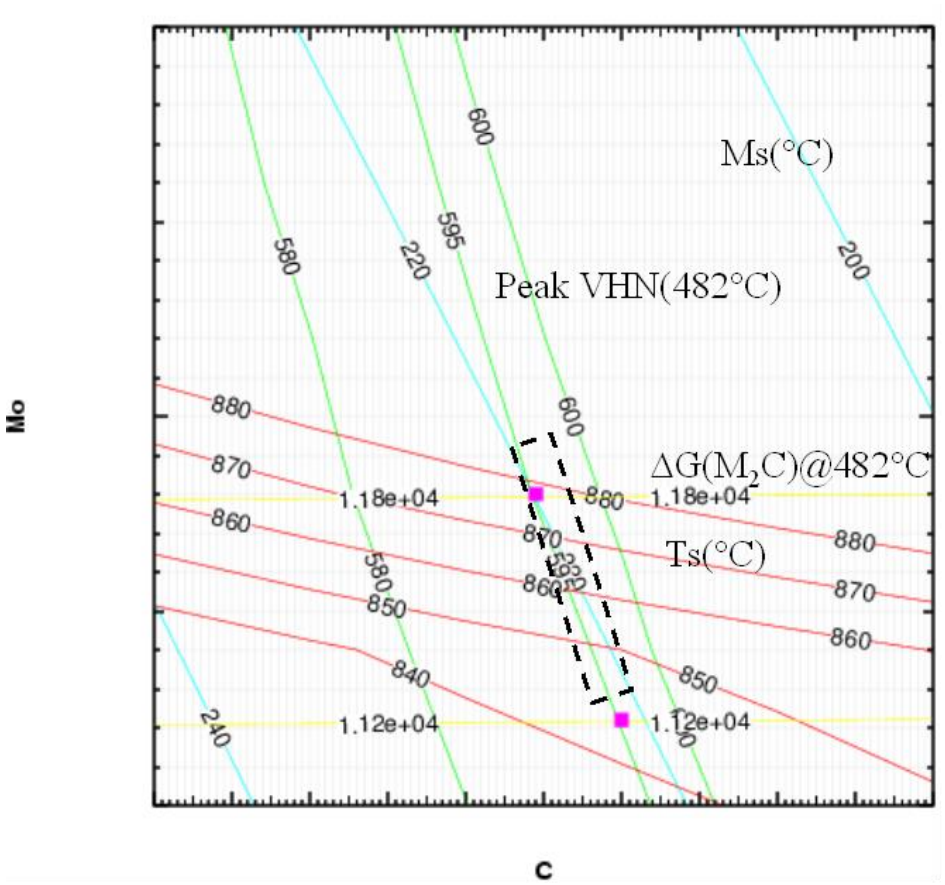
J.R. Rice and J.-S. Wang, Mater. Sci. Eng., 1988

W. T. Geng, A. J. Freeman and G. B. Olson, ***Phys. Rev. B*** 63 (2001) 165415.
W. Xiong and G. B. Olson, ***npj CompMat***, 2 (2016) 15009.

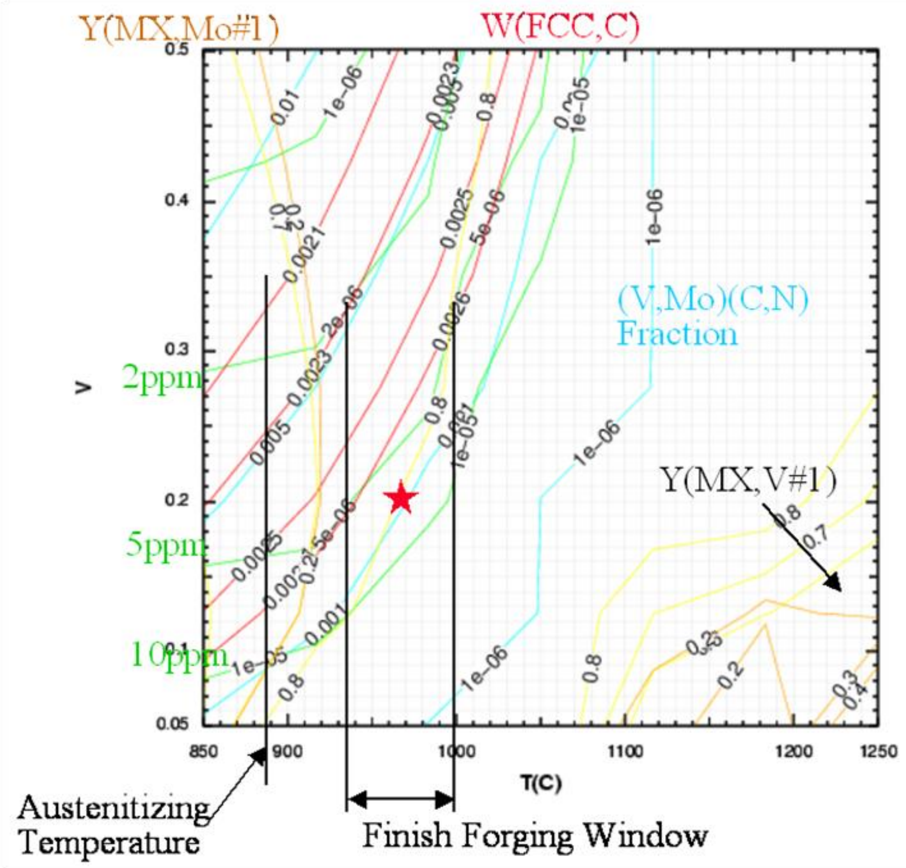


Example: Design Integration with CMD

Matrix + Strengthening Dispersion Design



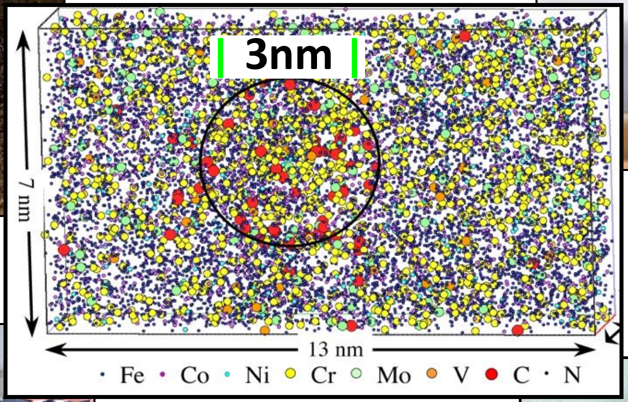
Grain Pinning Dispersion Design



CyberSteels to Market

QuesTek INNOVATIONS LLC

Ferrium C61 **AMS6517**



Ferrium S53 Stainless **AMS5922**

Ferrium C64 **AMS6509**

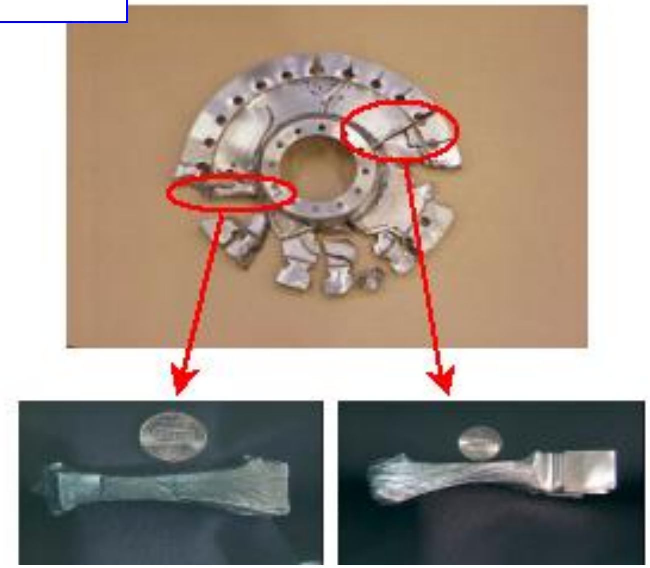
Ferrium M54 **AMS6516**

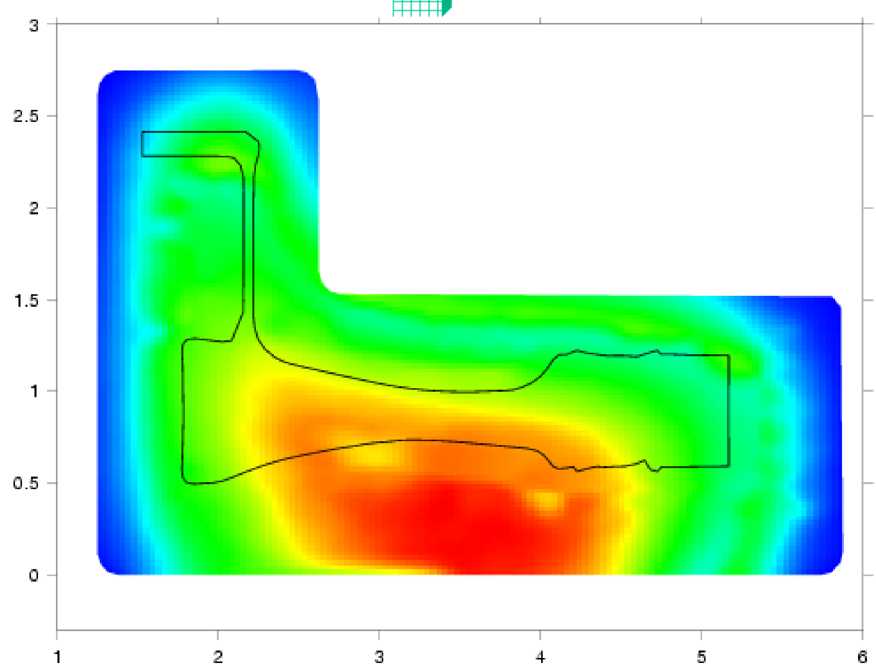
AUTOCOURSE
www.autocourse.com

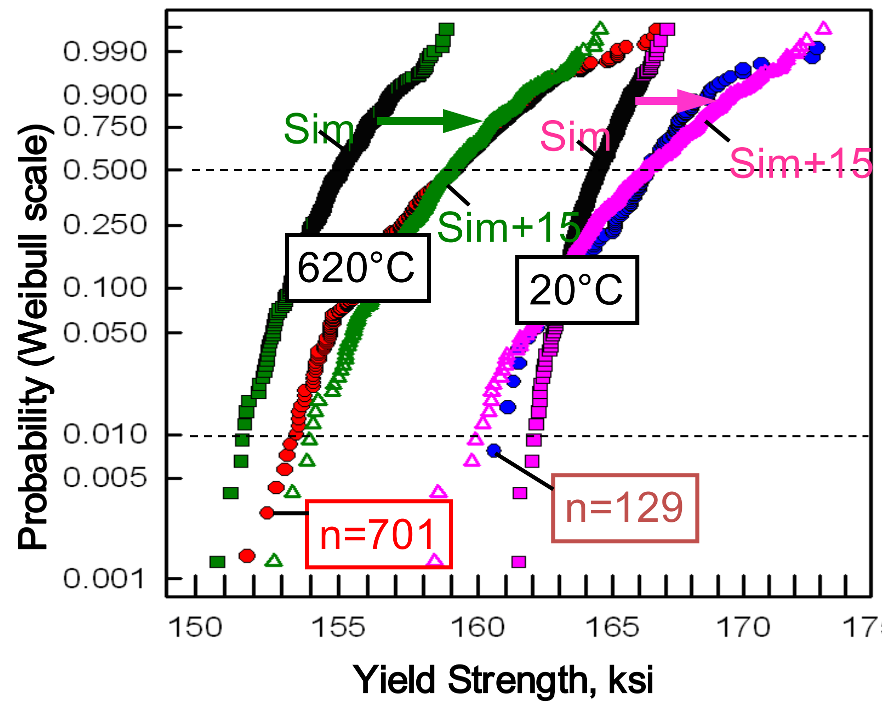
MAX VERSTAPPEN
Oracle Red Bull Racing

DARPA

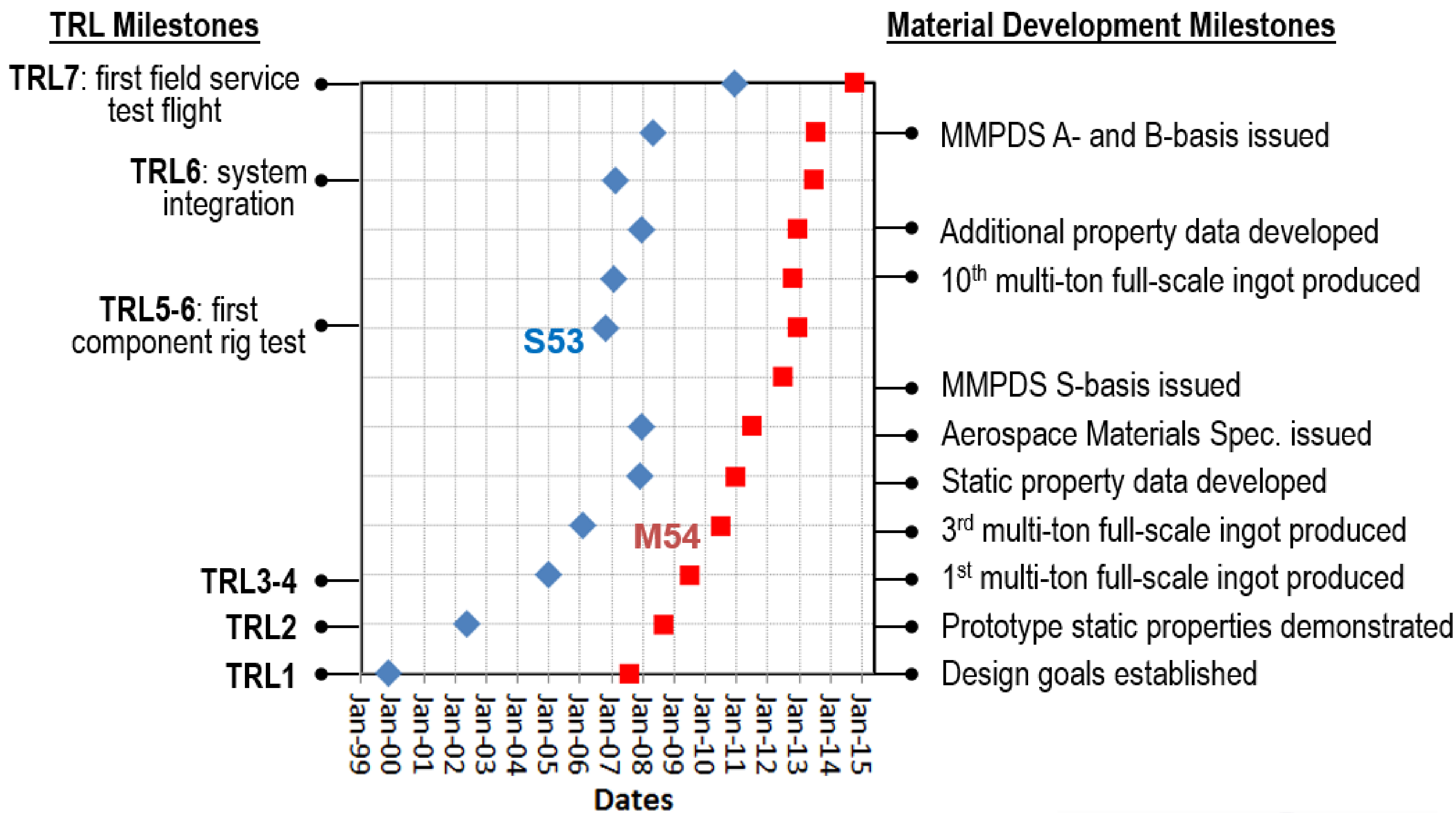
AIM Accelerated Insertion of Materials







Computational Materials Qualification Acceleration



QuesTek INNOVATIONS LLC

Apple watch

-Announced September 2014

Baseline: 316L Stainless Steel

-Cold-forged to 40% harder
-Special purity mirror finish

High Strength 18K Gold

-2X harder

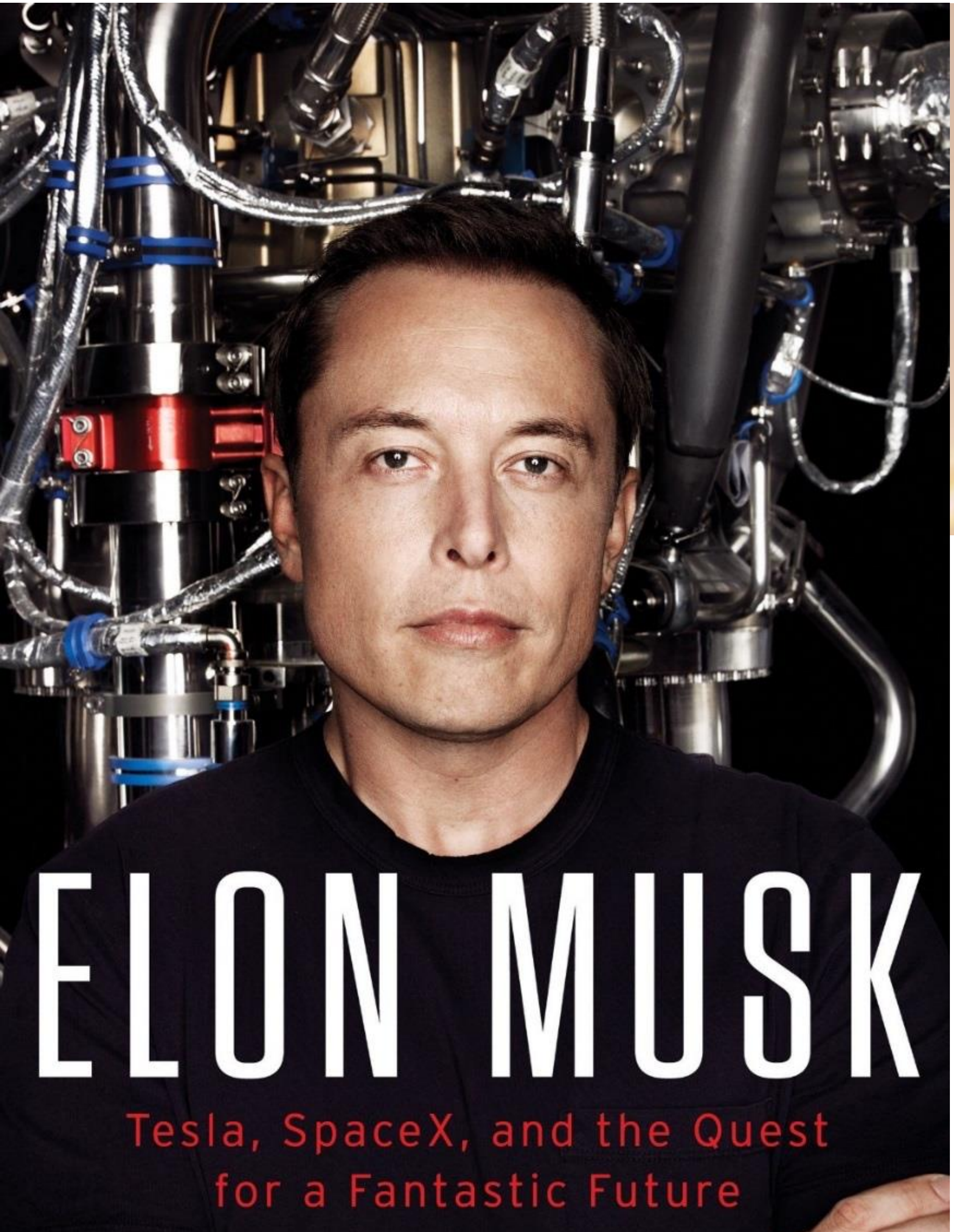
Milanese Loop Alloy

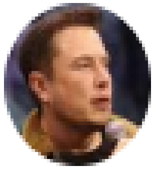
-Custom Magnetic Stainless Steel

Anodizable 7000 Aluminum

-60% stronger Al
-30% lighter than 316L

MGI: From Ferrium Ridge to Silicon Valley





Elon Musk
@elonmusk

Follow

Replying to @Robotbeat @Jon128123 and 8 others

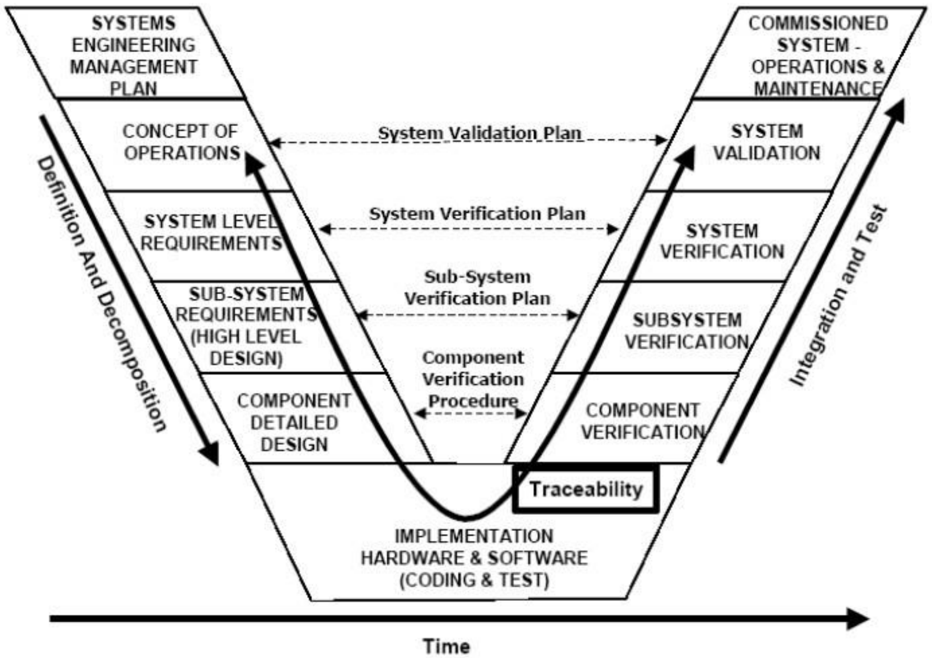
SpaceX metallurgy team developed SX500 superalloy for 12000 psi, hot oxygen-rich gas. It was hard. Almost any metal turns into a flare in those conditions.

7:40 PM - 22 Dec 2018

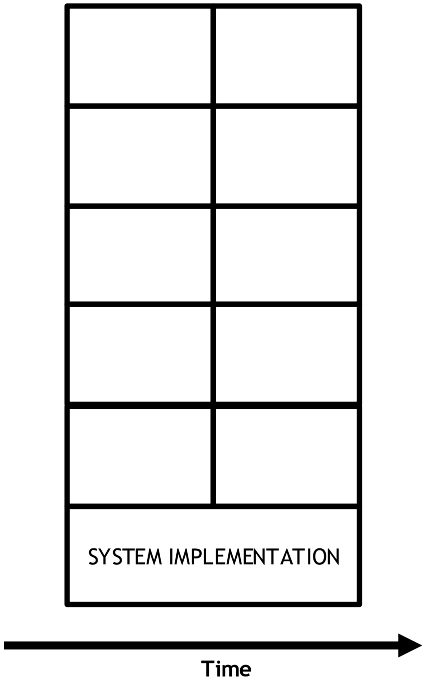
The Steel Starship

Manufacturing 5.0

Standard V-model for Systems Development Cycle



Total Concurrency



-After C. J. Kuehmann

The Algorithm

- *Step 1 – Question all requirements*
- *Step 2 - Delete the part or process*
- *Step 3 - Simplify*
- *Step 4 - Accelerate*
- *Step 5 - Automate*

SPACEX

NIST

CHiMaD

Center for Hierarchical Materials Design

- 10 yr $60M ($50M NIST + $10M cost match)
- Chicago Regional (Voorhees & Olson,**NU**/ dePablo,**UC** Founding Co-Directors)
- Methods, tools and databases supporting MGI; metals and polymers

NORTHWESTERN UNIVERSITY

THE UNIVERSITY OF CHICAGO

Argonne NATIONAL LABORATORY

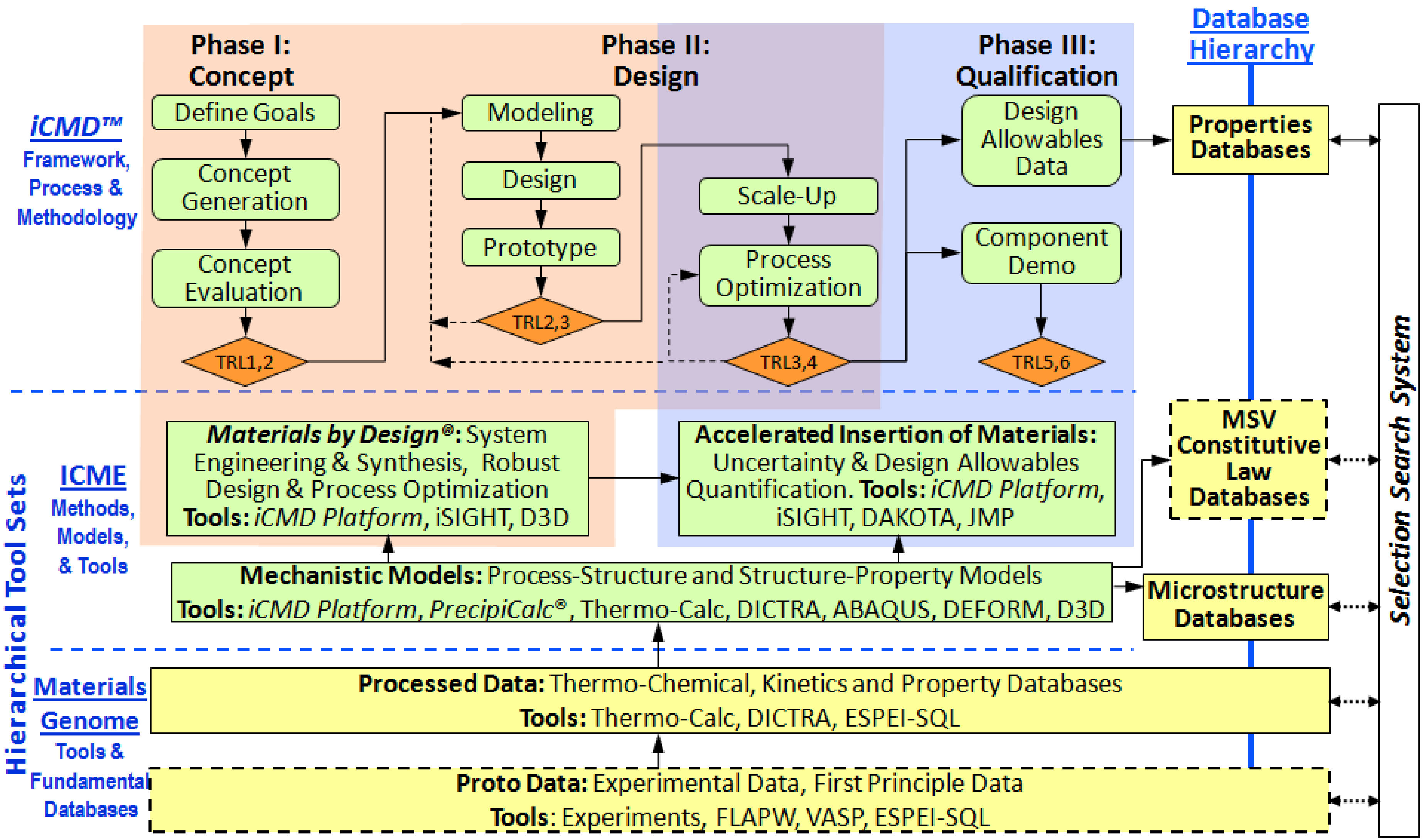
QUESTEK INNOVATIONS LLC

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

ASM MEF

CHiMaD

Center for Hierarchical Materials Design



CHiMaD Projects

Period 1: 2014-2018

Use-Case Groups:

- Precipitation-Strengthened Alloys
  - *(1) Co-base Superalloys*
  - *(2) High-Performance Shape Memory Alloys*
  - *(3) Precipitation-Strengthened Thermoelectrics*
- In-Situ Silicon Composites
- Low-Dimensional Nanoelectronic Materials
- Polymer Matrix Materials for Composites
- Directed Self-Assembly of Block Co-Polymer Films for Lithographic Applications
- Soft-Matter Design Based on Charge Complexation
- Organic Bulk Heterojunction Polymer Solar Cells

Seed Groups:

- Additive Manufacturing
- Impact Mitigation

Tool Groups:

- Materials Data Facility
- Phase Field
- Data Mining
- Metals Processing Facility

Period 2: 2019-2023

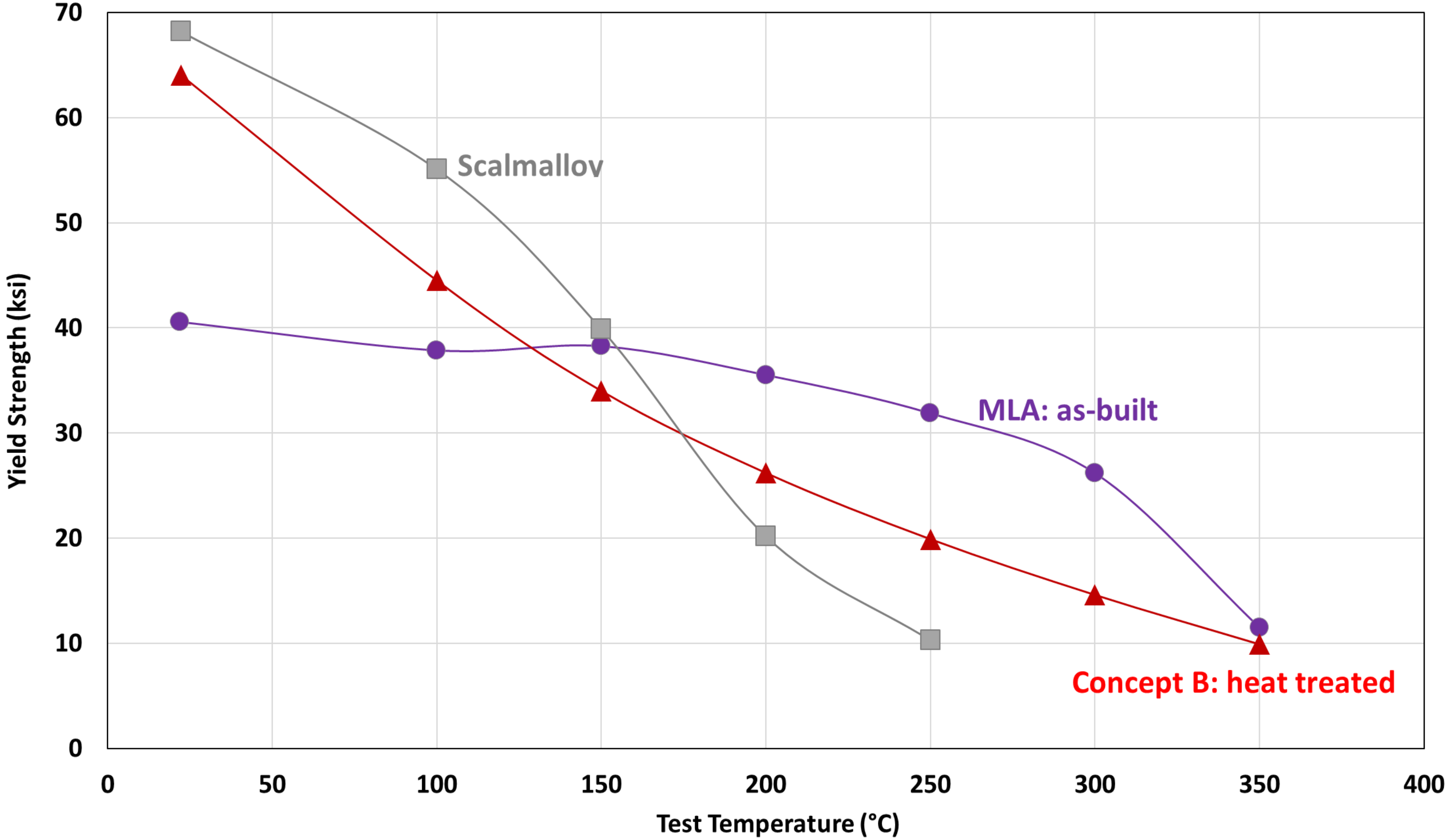
Use-Case Groups:

- Accelerated Development of Cobalt-Based Superalloys for High-Temperature
- Alloy Design for Additive Manufacturing
- Two-Dimensional Electronic Material Inks
- Grain Boundary and Interface Engineering in Thermoelectrics
- Directed Self-Assembly (DSA) of Soft Matter Systems
- High Performance Composite Design for Extreme Environments
- Material Design for High-Performance Impact Protection
- Design of Static and Dynamic Properties of Polyelectrolyte Complexes

Tool Groups:

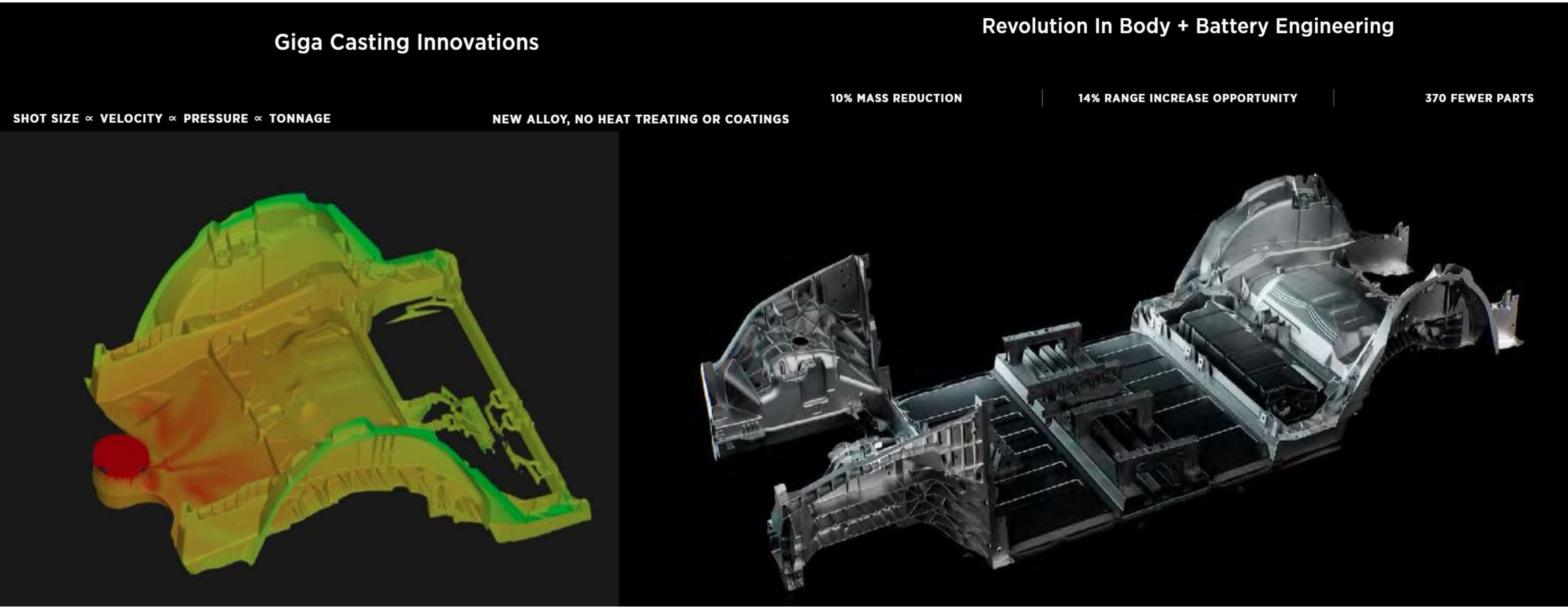
- Data Mining & Analytics Tools
- Quantitative Phase Field Modeling
- Materials Data Facility
- Uncertainty Quantification of Phase Equilibria and Thermodynamics

HT Aluminum for AM

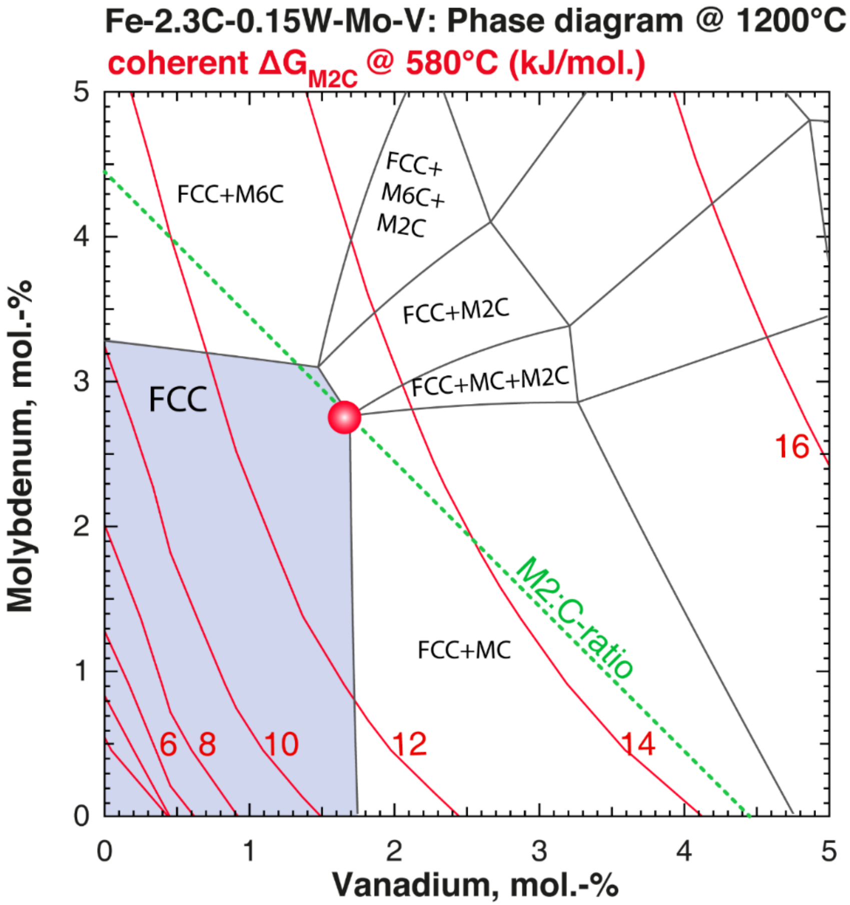


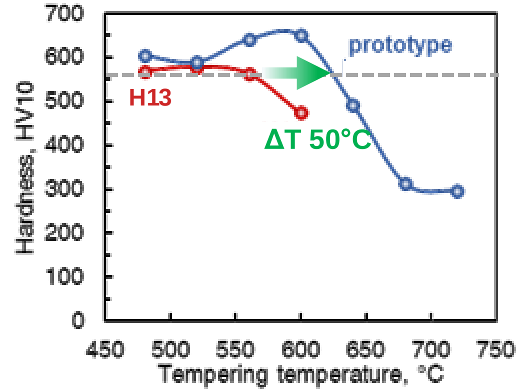
QuesTek® INNOVATIONS LLC

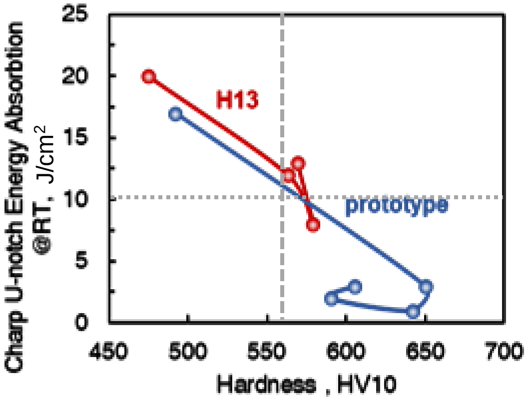
Tesla’s Giga Casting Aluminum



Printable GigaCasting Die Steels







Tesla creates new team to accelerate use of new materials in its products

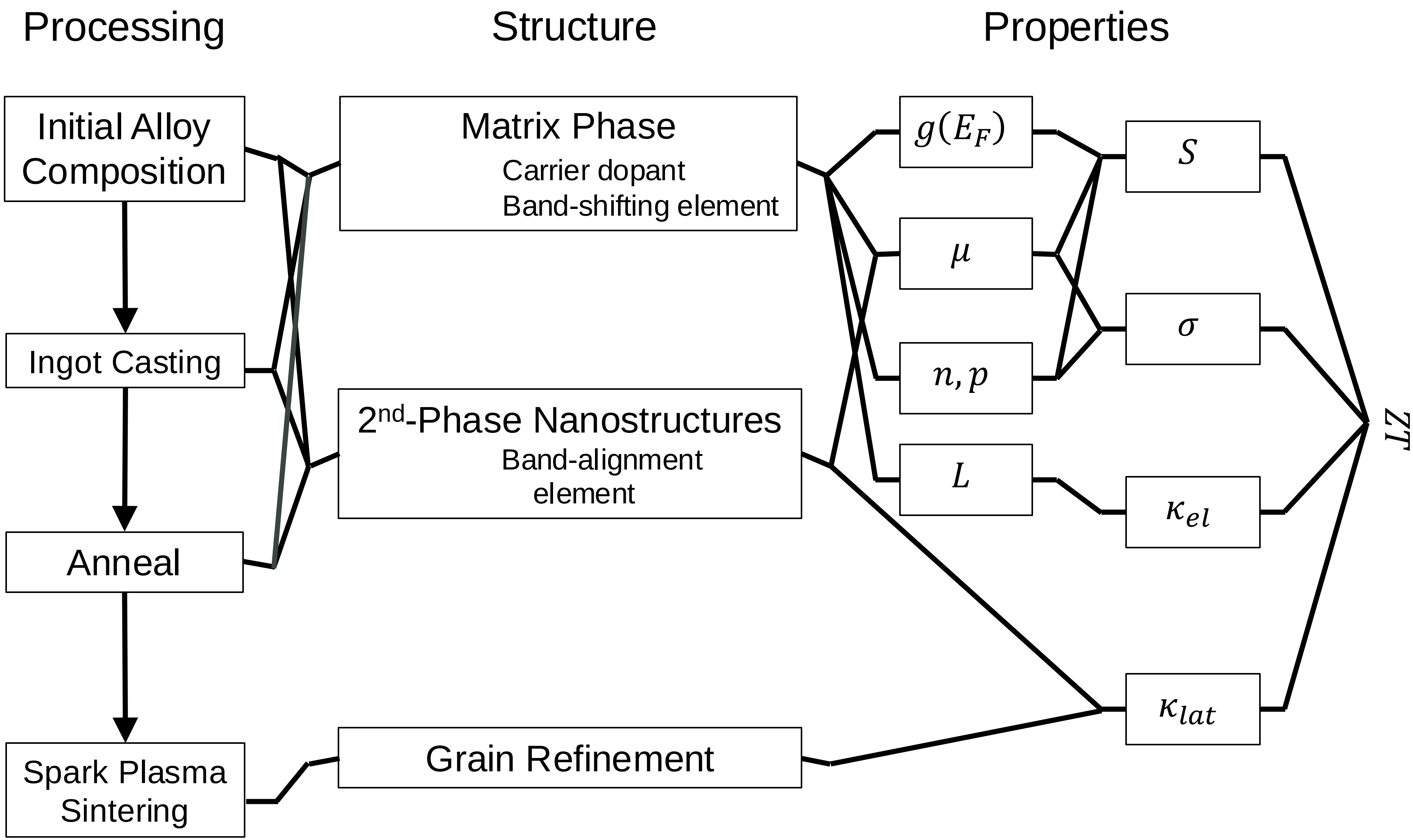
- Tesla's Charles Kuehmann created a new cross-company material engineering team to design new advanced materials
- A new materials applications team at Tesla has also been created to help integrate the new materials more rapidly
- *"The idea is to accelerate the adoption of new materials and processes – helping to bridge the gap between materials science and part design"* David Nelson, Tesla Drive System Engineering

https://electrek.co/2021/04/22/tesla-creates-new-team-accelerate-use-materials-products/

DARPA-SIMPLEX:
Data-driven Discovery for Designed Thermoelectric Materials

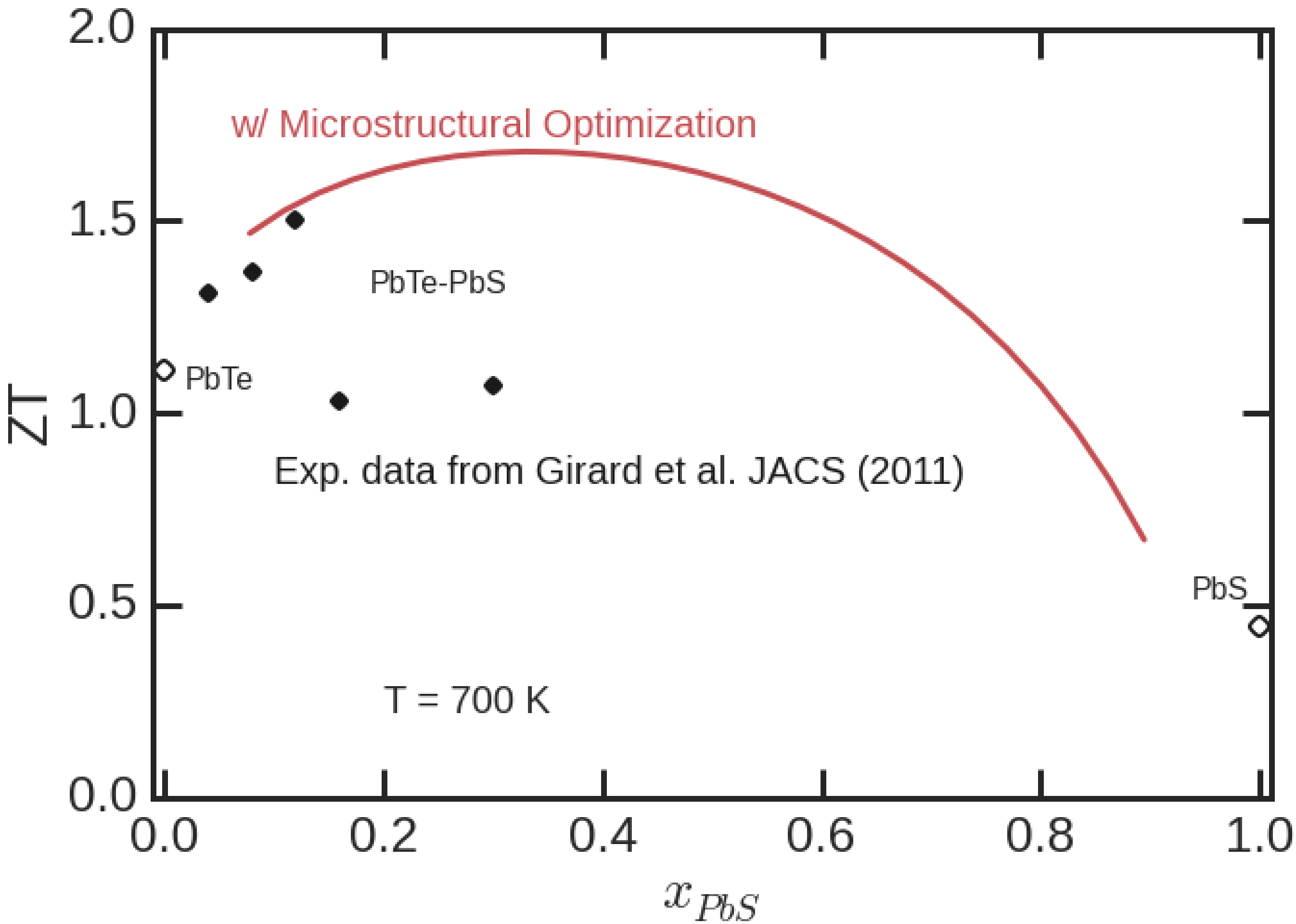
G. B. Olson, PI
James Saal, Project Coordinator

Thermoelectric Materials Design

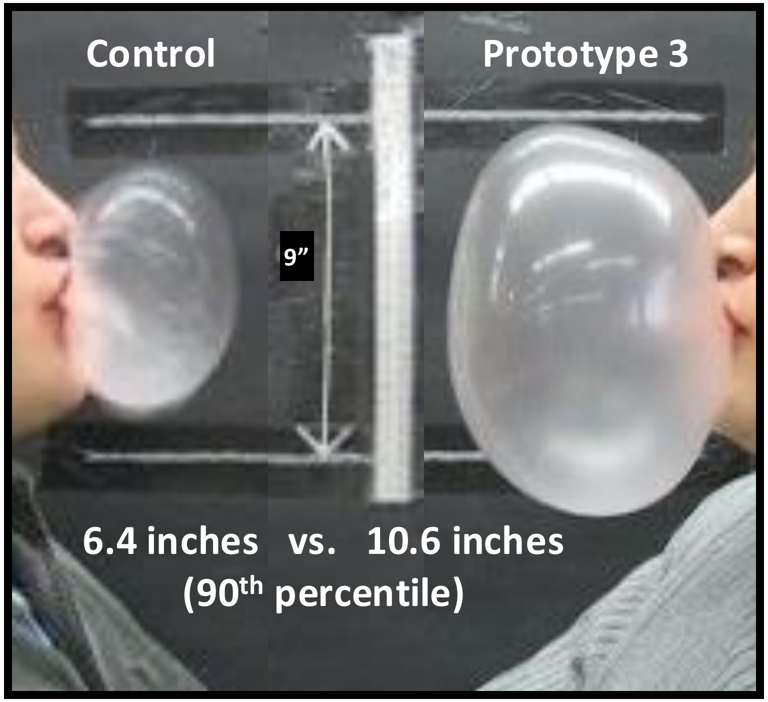


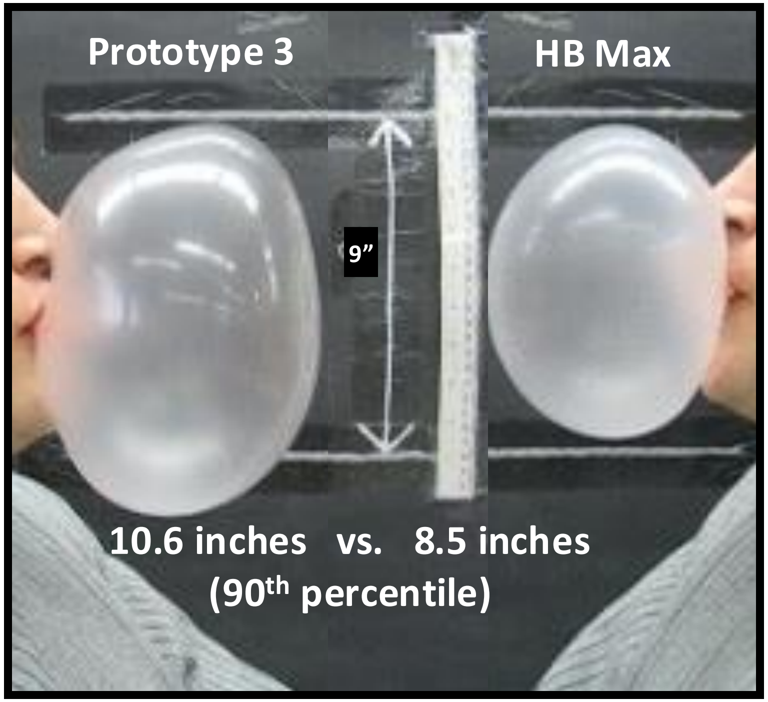
Microstructural Control of Lattice Thermal Conductivity

Predicted 13% improvement in ZT achievable
with particle refinement at optimum phase fraction



Applied Amorphensite: SuperGum (2008 Undergraduate Design Competition)





3.041/3.321 Computational Materials Design

Spring 2024
Design Projects

I. Printable Co Superalloy (ASM)

Client: P&W (Dr. Dave Furrer); NIST-CHiMaD
Advisor: Krista Biggs, Dr Julio Dos Santos
Team: Marilyn Meyers, Charles Yong; Michelle Zong (UROP)

II. 10Ni Transformation-Toughened Naval Hull Steel

Client: OSD (Dr. Matt Draper); ONR
Advisor: Cole Kuehmann
Team: Aayushi Chauhan, Takuji Otake, Ryuichi Suehiro

III. Fatigue Resistant SUS301-EH

Client: Apple (Dr Zack Feinberg)
Advisors: Brandon Snow, Julian Rackwitz
Team: Bill Liu, Killian Sheriff

IV. Printable GigaCasting Tool Steel

Clients: Tesla (Chris Kern); SpaceX (Dr Jim Wright); DOE-AMO
Advisor: Dr. Florian Hengsbach, U Paderborn
Team: Stanley Chang, Gary Whelan

V. CABLE Twitchalloy: HS/HC/HT Aluminum Alloy

Client: Constellium (Dr. Laurent Boissonnet)
Advisor: Dr. Margianna Tzini
Team: Constantine Athanitis, Hao Tang

SRG 3.0

CyberSteels: Accelerating Genomic Design

December 2022 start; Duration 7 years

1. Simulation-Based Design

G. B. Olson (DMSE): Design Integration

D. M. Parks (DME): Multiscale Transformation Toughening Simulation

E. A. Olivetti* (DMSE): Economic Model Integration

2. Mapping the Steel Genome

2.1 *The GB Genome*

C. A. Schuh/R. Freitas (DMSE): Pseudopotential DFT

J. C. Grossman* (DMSE): All-electron DFT, Bond Topology

C. C. Tasan (DMSE): Advanced SEM

J. M. LeBeau* (DMSE): STEM Microanalysis

2.2 *The L Genome*

A. Allanore (DMSE): Thermophysical Measurements

Excelsior

Backup Slides

MSc390 Materials Design

Spring 2019
Design Projects

I. Ferritic Superalloy

Client: NSF
Advisor: Yao Du
S. Bohle*, D. Kostelancik, K. Sugiyama*

II. 3D Printing TRIP Steel (ICME)

Client: NIST-CHiMaD, DMDII, QuesTek
Advisor: Clay Houser
J. Hechter, R. Pee, S. Sorkin, S. Webster

III. HP Shape Memory Alloy

Client: NIST-CHiMaD, QuesTek
Advisor: Chuan Liu
T. Cote, S. Ruiz, K. Su

IV. Co Superalloy

Client: NIST-CHiMaD, QuesTek
Advisor: Dr. Jiadong Gong, Dr. Peisheng Wang
M. Alzayer, L. Borgsmiller, J. Pieterse, C. Wolff

V. 3D Printing TRIP Titanium

Client: NIST-CHiMaD, DMDII, ONR, QuesTek
Advisor: Fan Meng
Z. Liang*, R. Orenstein, D. Zhang

VI. High ZT Thermoelectric

Client: DARPA-MATRIX,NIST-CHiMaD,QuesTek
Advisor: James Male
W. Jeang, M. Paul, G. Young

3.041/3.321 Computational Materials Design

Spring 2020
Design Projects

I. Printable TRIP Steel (ASM)

Client: NIST-CHiMaD, ONR

Advisor: Clay Houser

II. Printable PH Shape Memory Alloy

Client: NIST-CHiMaD

Advisor: Chuan Liu

III. Printable High-T Aluminum

Client: NIST-CHiMaD, DLR-Germany

Advisor: Florian Hengsbach

IV. TRIP Zirconia Ceramics

Client: NSF, ARO

Advisor: Edward Pang

3.041/3.321 Computational Materials Design

Spring 2021
Design Projects

I. Printable Co Superalloy

Client: NIST-CHiMaD
Advisor: Dr. Chuan Liu
Team: Yannick Naunheim, Noriaki Arai*

II. HSLA150: Transformation-Toughened Naval Hull Steel

Client: NIST-CHiMaD, ONR, SPI
Advisor: Clay Houser
Team: Julian Rackwitz, Brandon Snow

III. Lead-Free Solder

Client: Apple (Dr. Zack Feinberg)
Advisor: Edward Pang
Team: Spencer Hu, Nutth Tuchinda

IV. Printable Tool Steel

Client: NIST-CHiMaD, U Paderborn
Advisor: Florian Hengsbach
Team: Krista Biggs, Gary Whelan*

V. UHS Al Plate Alloy

Client: DSO-Singapore
Advisor: Dr. Margianna Tzini
Team: Alvin Tan, Jonathan Lim, Huan-Chin Koh, Wei-Lin Tan

3.041/3.321 Computational Materials Design

Spring 2022
Design Projects

I. Printable Co Superalloy
Client: NIST-CHiMaD
Advisor: Krista Biggs
Team: Christopher Kiel, Ben Graybill

II. Printable GigaCasting Die Steel (ASM)
Client: Tesla (Dr. Quin Hamill)
Advisor: Florian Hengsbach*, U Paderborn
Team: Ian Chen, Kyle Markland

III. Mars StarShip Steel
Client: SpaceX (Dr. Jim Wright)
Advisors: Brandon Snow, Julian Rackwitz
Team: Sam Song, Myles Stapelberg

IV. UHS Al Plate Alloy
Client: DSO-Singapore
Advisor: Dr. Margianna Tzini*
Team: Luca Montinelli, Elliott Yarwood, Peiwen Ren*

Question and Answer Session

Dr. Clive Freeman

Materials Design

Professor Greg B. Olson

MIT and QuesTek Innovations, LLC

Announcements

ugm.materialsdesign.com

MedeA Training

Thursday, October 24th

Dr. Xiaoli Liu

Materials Design

Next Week's Plenary Session

Tuesday, October 29th

Professor Sir Richard Catlow

University of College London

Question and Answer Session

Dr. Clive Freeman

Materials Design

Professor Greg B. Olson

MIT and QuesTek Innovations, LLC

Questions about Materials Design UGM

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MedeA

Innovation by Simulation