Genomic Materials Design: From CALPHAD to Flight

G.B. Olson[1,2] & Jason Sebastian[2]

1.Northwestern University

2.QuesTek Innovations LLC

Evanston, Illinois

NORTHWESTERN UNIVERSITY

CHiMaD

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)

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**

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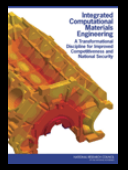
Materials Genome Timeline

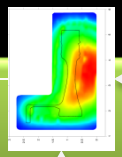
2004 NMAB Accelerating Technology Transition

2008 NMAB ICME



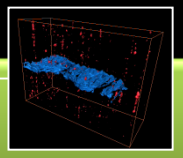
2011 OSTP

2001 DARPA AIM



2003 Ford VAC

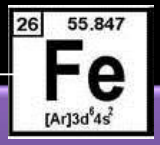
2005 ONR/DARPA D3D



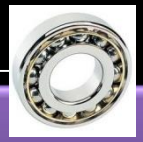
Concurrent Engineered Systems

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

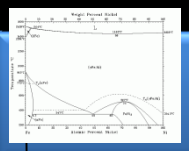
Refractories

SMAs
Al-base Alloys

Cu-base Alloys

PrecipiCalc®

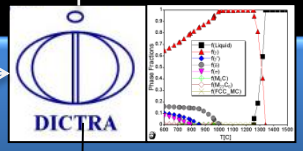
Materials Genome



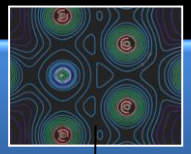
1956
Kaufman & Cohen

1973
CALPHAD

1979-84
Thermo-Calc
SGTE



1990s
DICTRA
Pandat
Thermotech



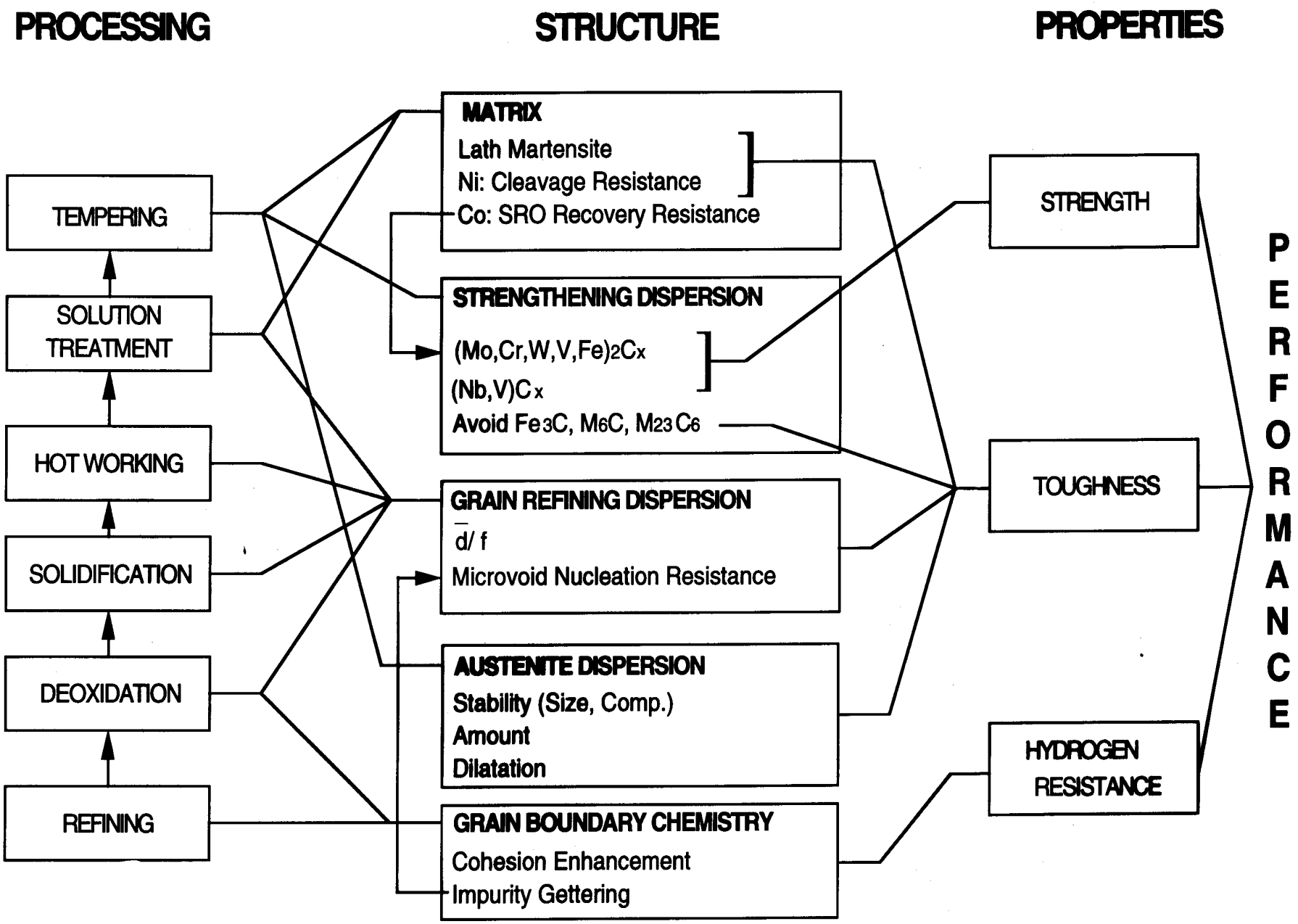
2000s
DFT Integration

2011
Materials
Genome
Initiative

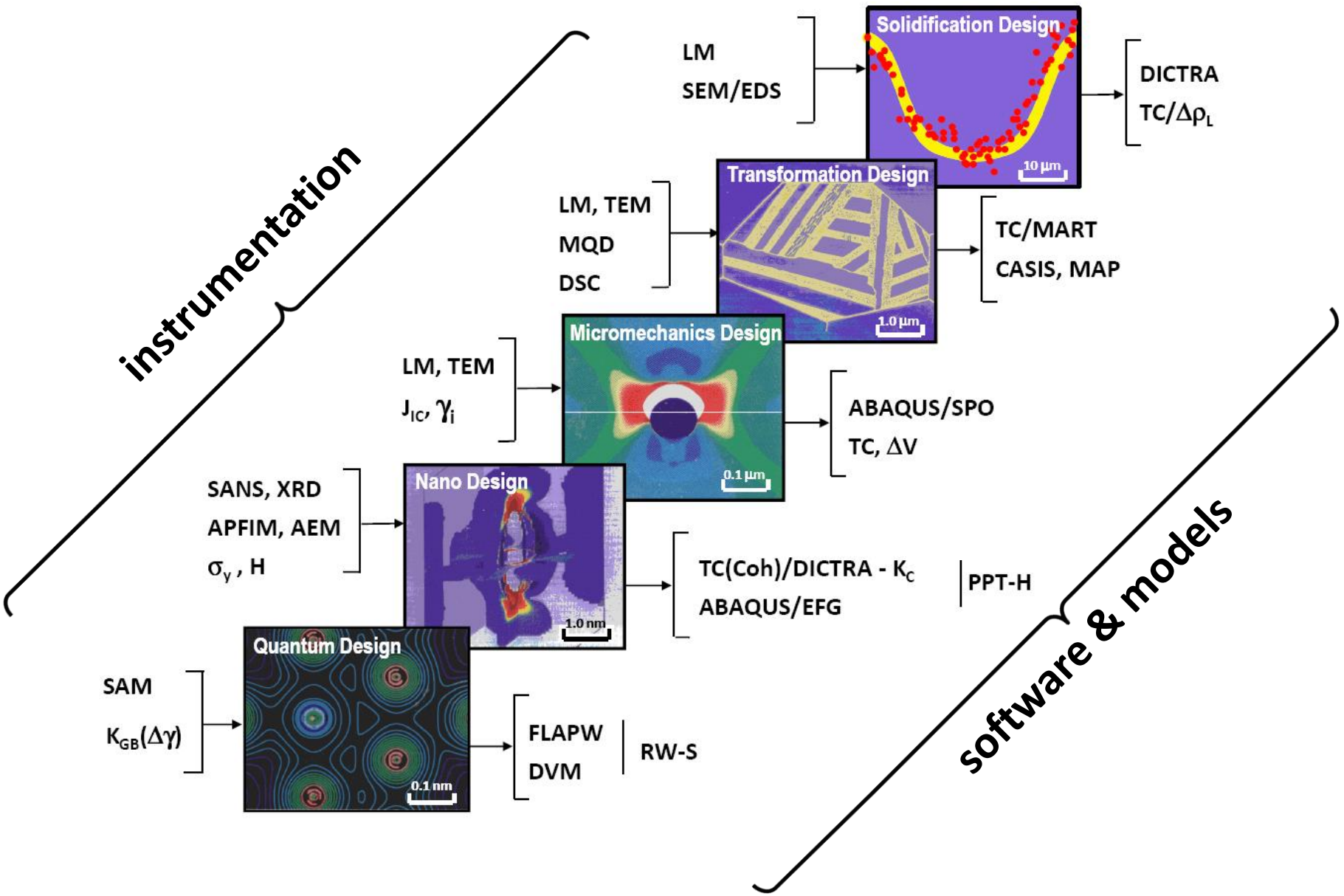
Gen I
1950
1970

Gen II
1980
1990
2000

Gen III
2010

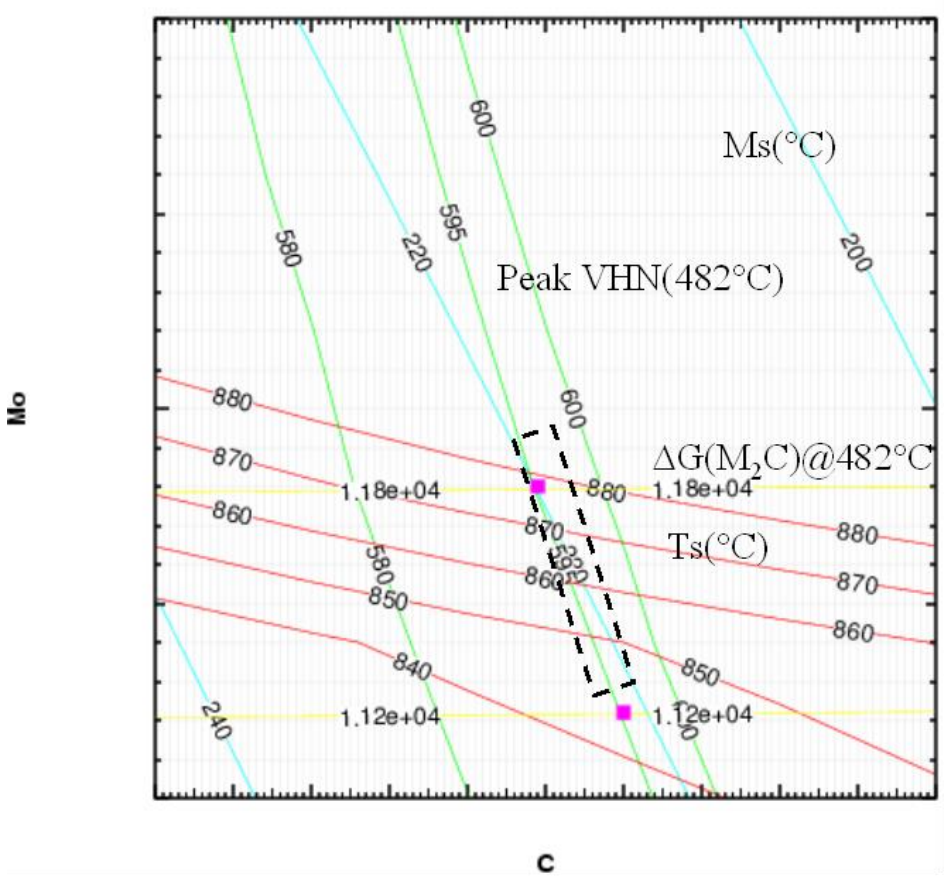

PROCESSING
STRUCTURE
PROPERTIES
TEMPERING
SOLUTION TREATMENT
HOT WORKING
SOLIDIFICATION
DEOXIDATION
REFINING
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
STRENGTHENING DISPERSION
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
GRAIN REFINING DISPERSION
d̄/ f
Microvoid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

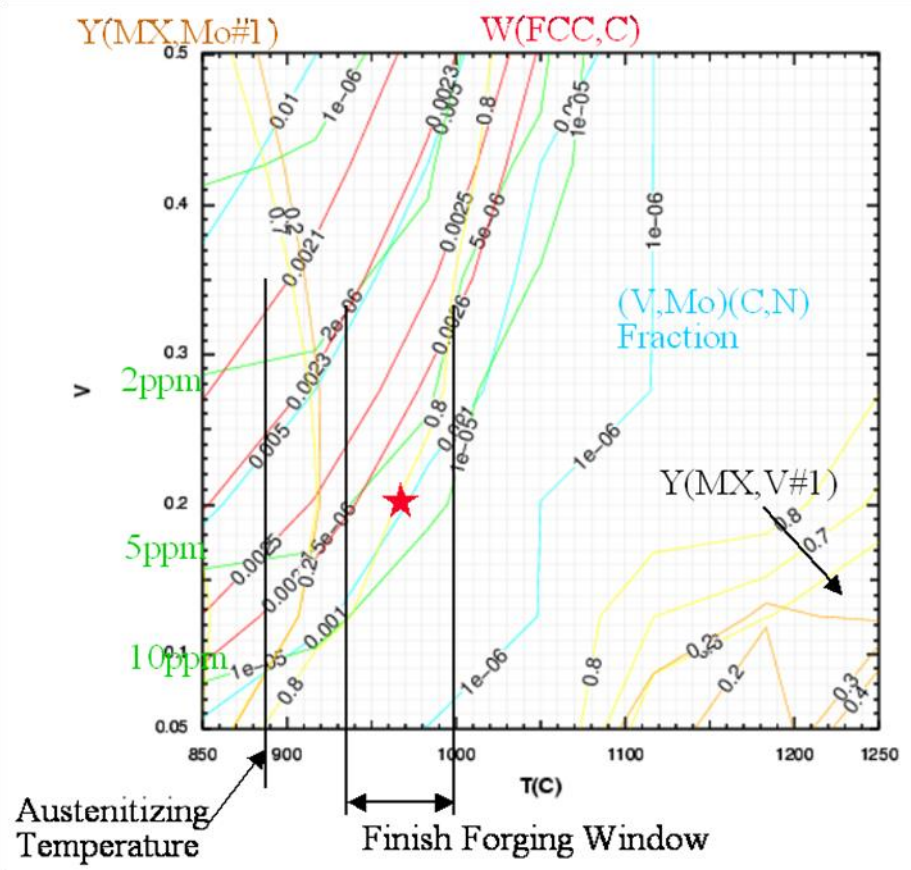


Example: Design Integration with CMD

Matrix + Strengthening Dispersion Design



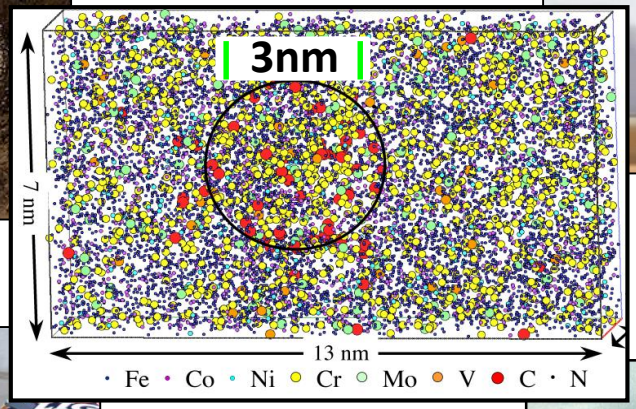
Grain Pinning Dispersion Design



CyberSteels to Market

QuesTek® INNOVATIONS LLC

Ferrium C61 **AMS6517**



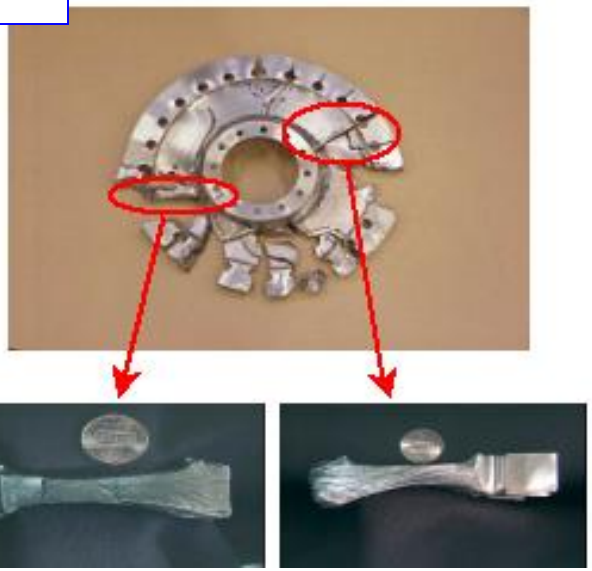
Ferrium S53 Stainless **AMS5922**

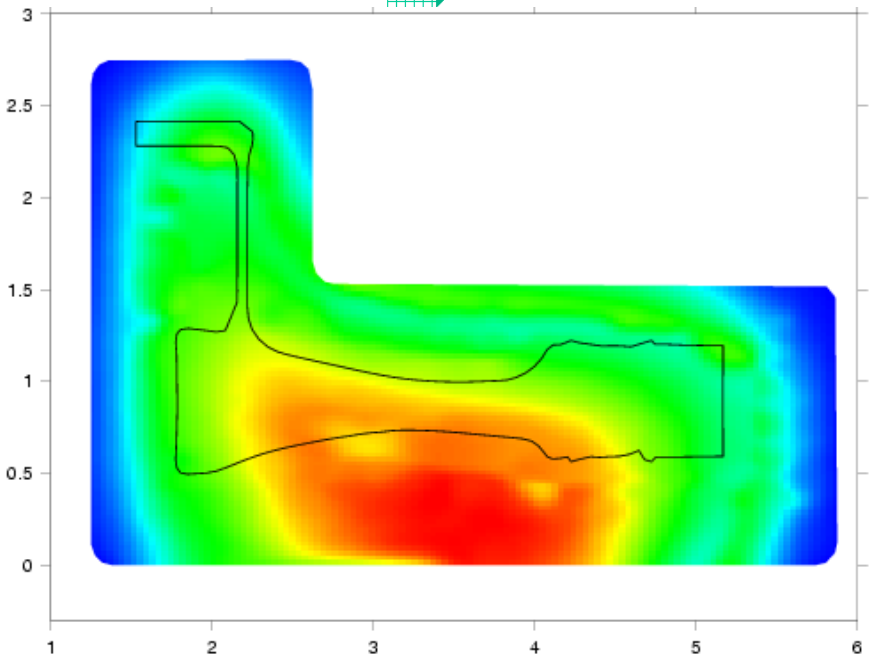
Ferrium C64 **AMS6509**

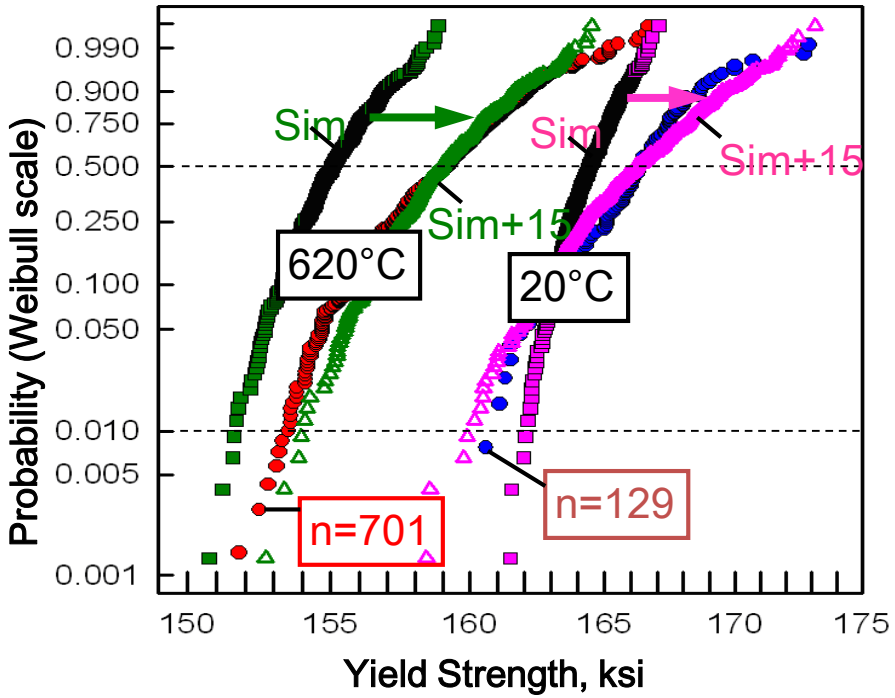
Ferrium M54 **AMS6516**

DARPA

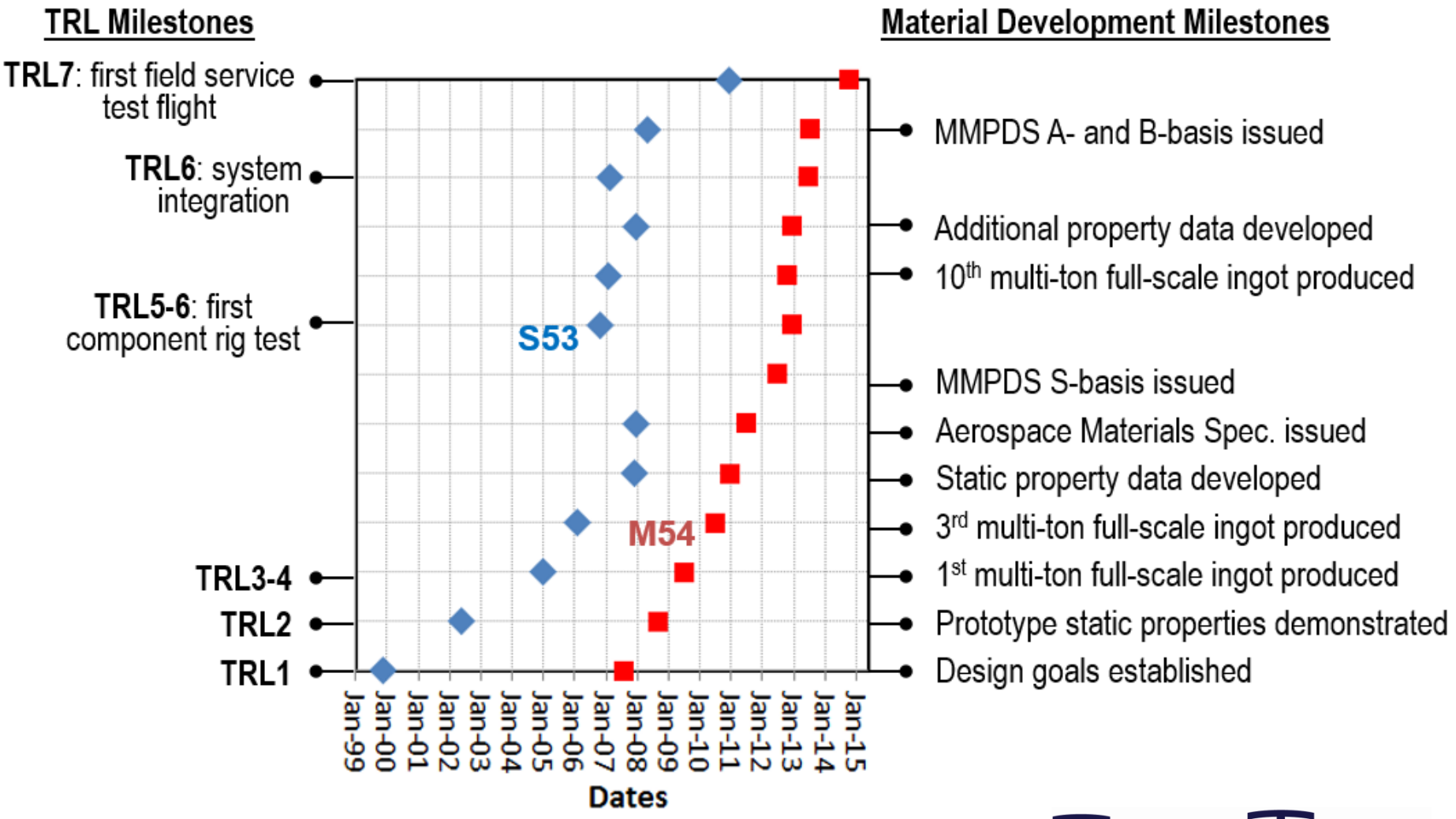
AIM
Accelerated Insertion of Materials







Computational Materials Qualification Acceleration



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Apple watch

-Announced September 2014

Baseline: 316L Stainless Steel

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

High Strength 18K Gold

-2X harder

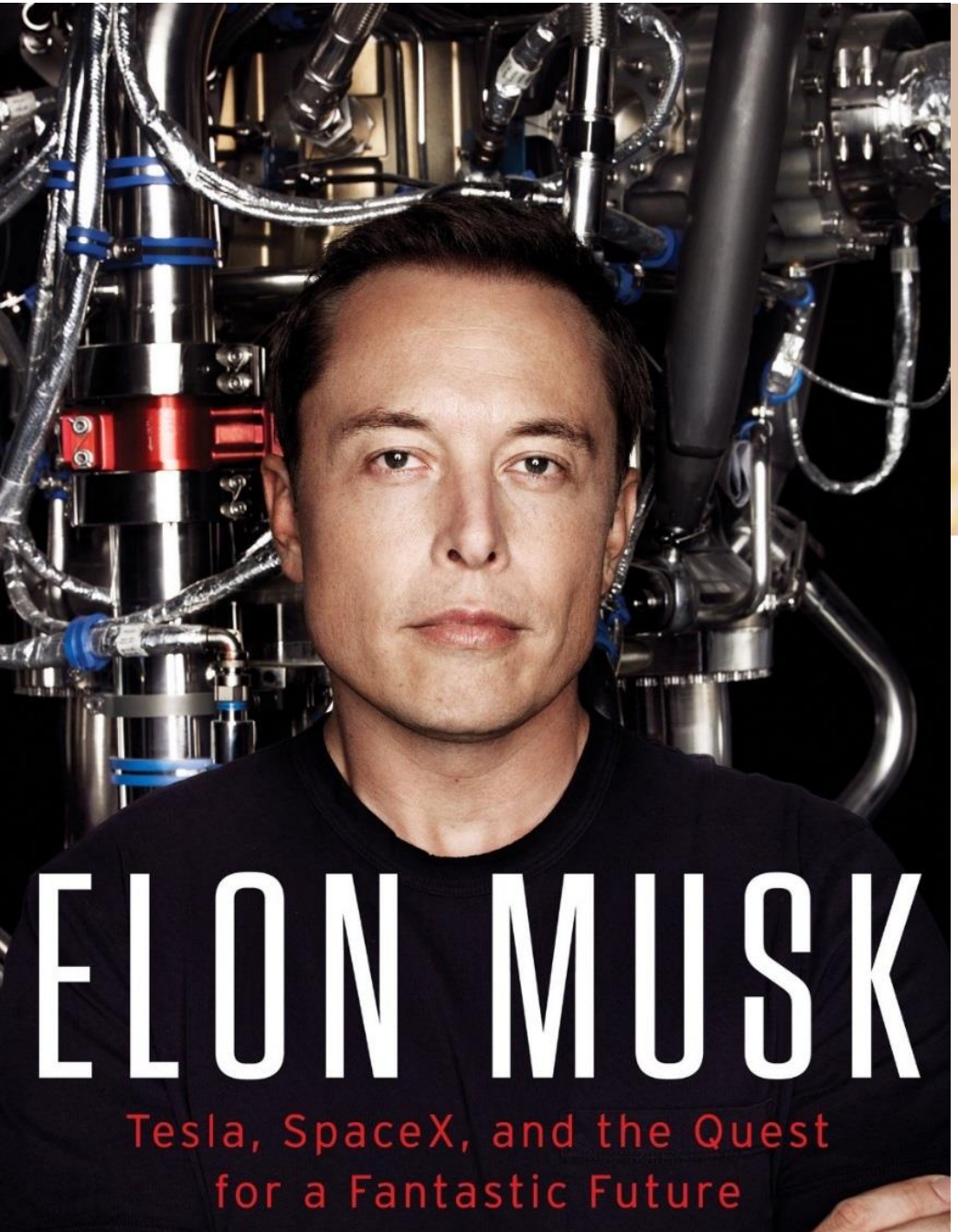
Milanese Loop Alloy

-Custom Magnetic Stainless Steel

Anodizable 7000 Aluminum

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

MGI: From Ferrium Ridge to Silicon Valley



Elon Musk

@elonmusk

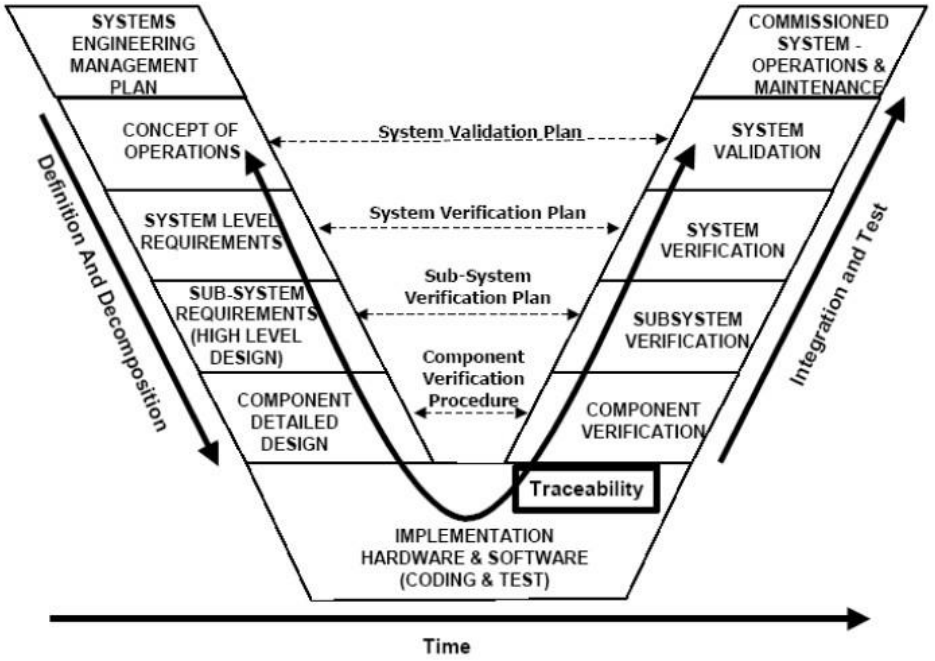
Follow

Replying to @Robotbeat @Jon128123 and 8 others

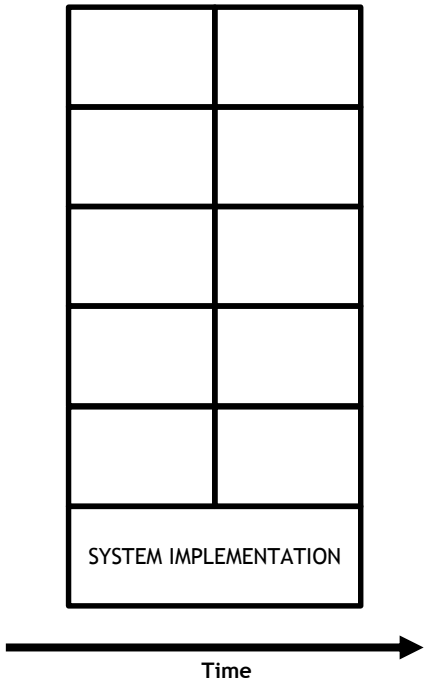
SpaceX metallurgy team developed SX500 superalloy for 12000 psi, hot oxygen-rich gas. It was hard. Almost any metal turns into a flare in those conditions.

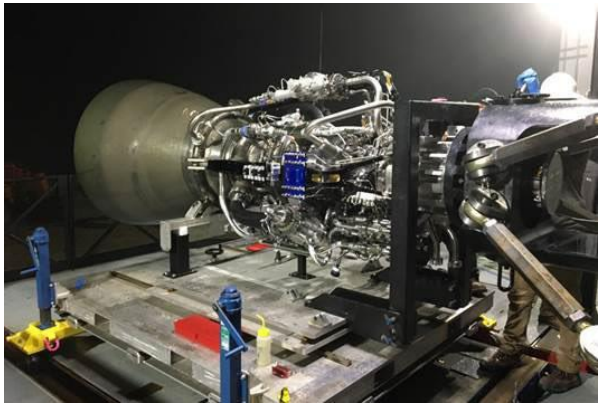
7:40 PM - 22 Dec 2018

Standard V-model for Systems Development Cycle



Total Concurrency





NIST

CHiMaD

Center for Hierarchical Materials Design

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

NORTHWESTERN UNIVERSITY

THE UNIVERSITY OF CHICAGO

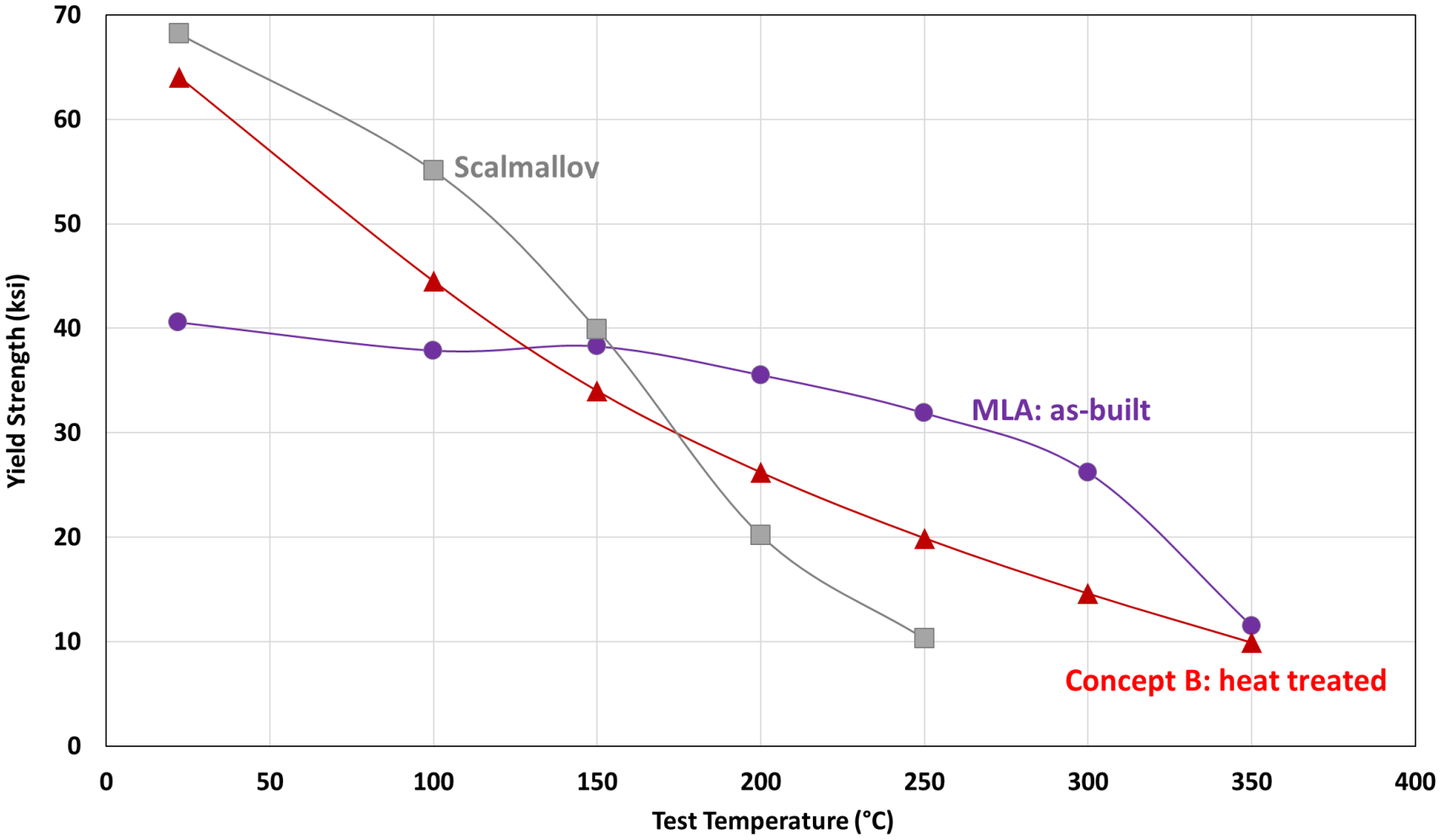
Argonne NATIONAL LABORATORY

QUESTEK INNOVATIONS LLC

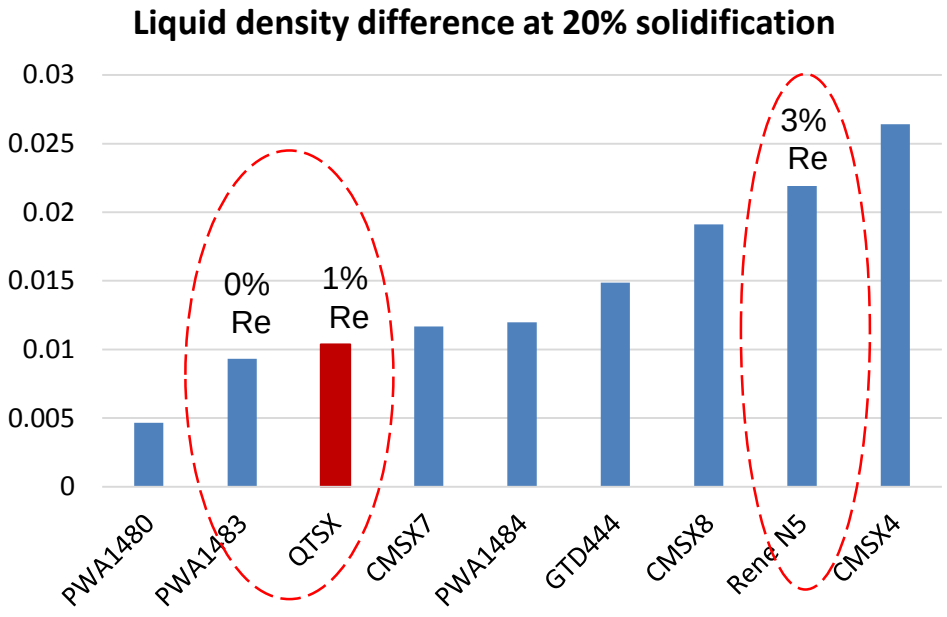
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

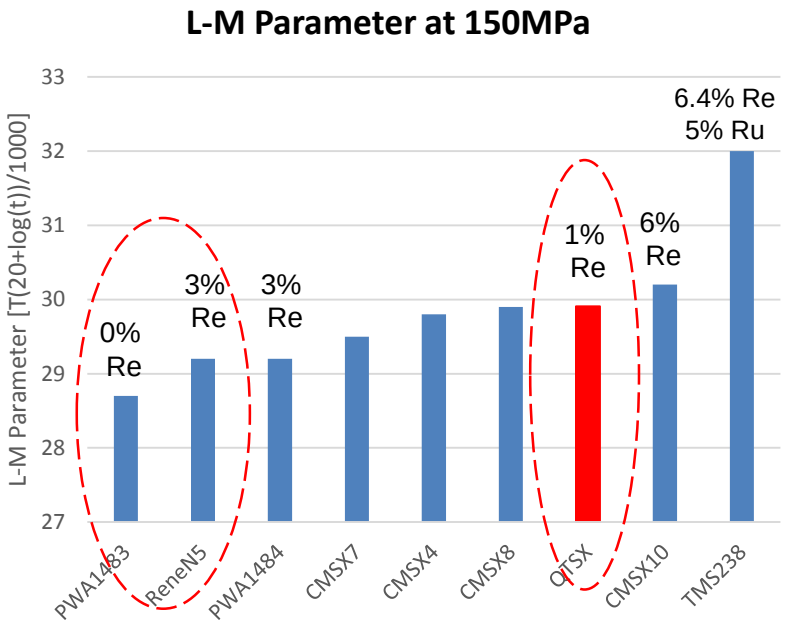
ASM INTERNATIONAL

HT Aluminum for AM



QTSX 1Re IGT SX Ni Superalloy
-Processability & Performance





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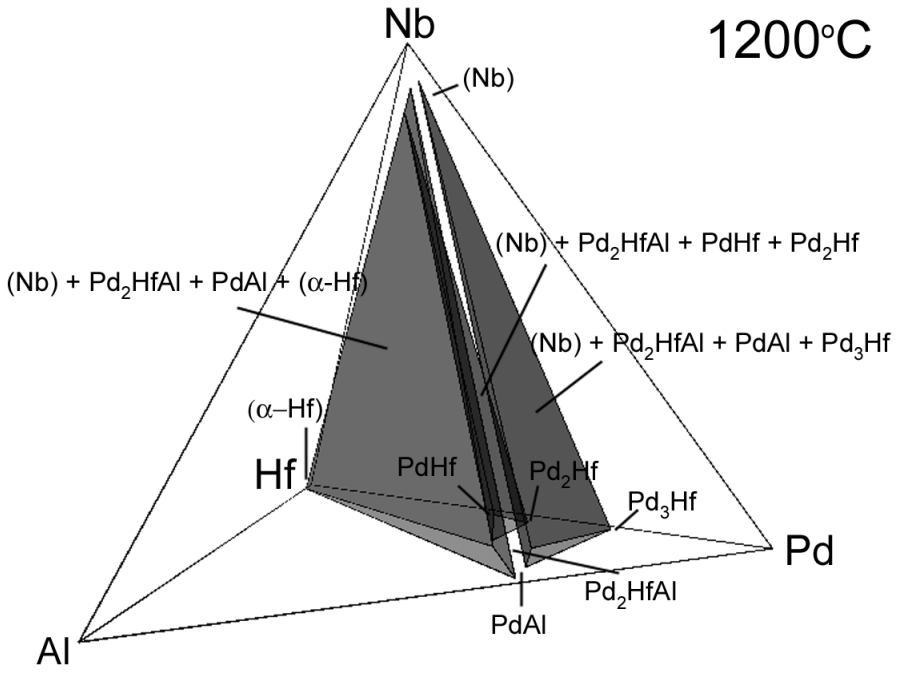
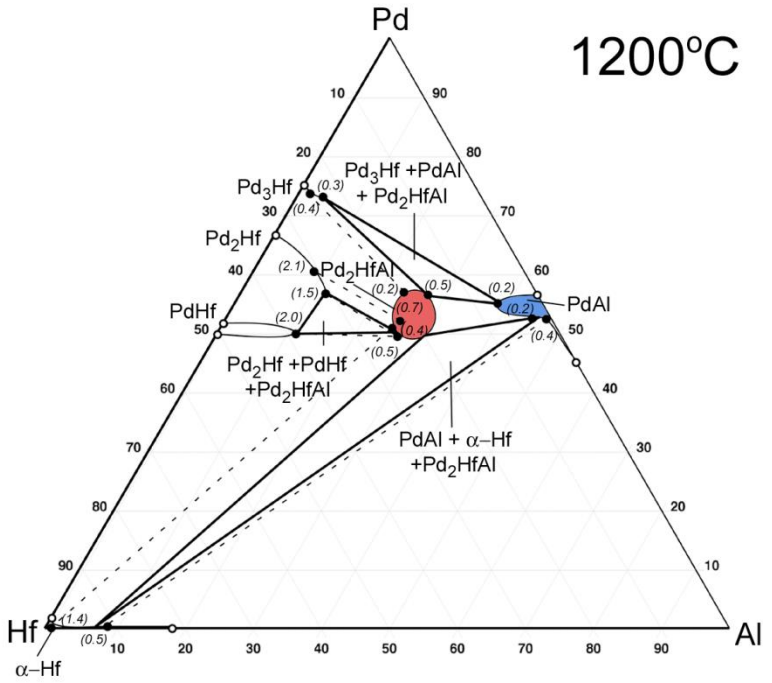
Al_2O_3 Concept

Nb-Pd-Hf-Al Phase Diagram





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

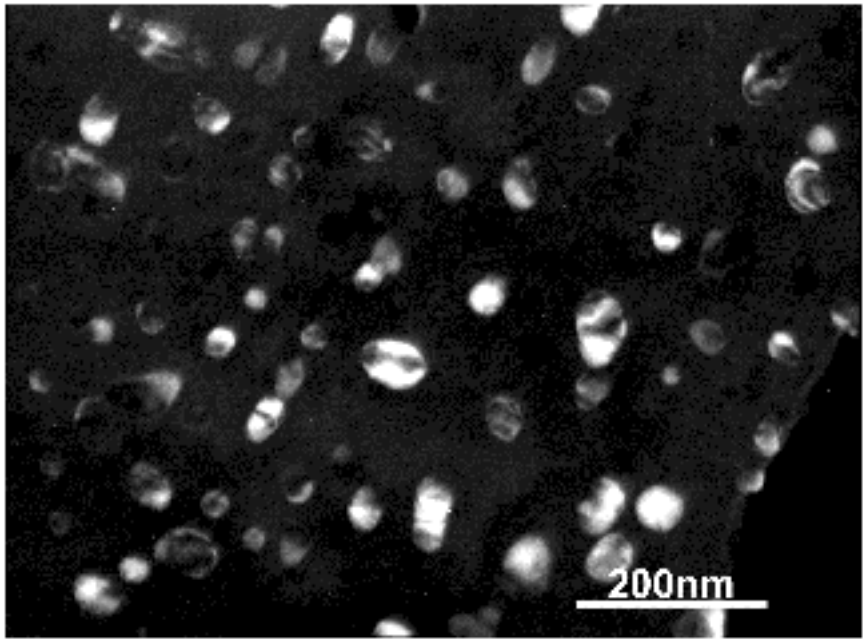
Projection of Nb-Pd-Hf-Al tie-tetrahedra bases on **Pd-Hf-Al plane** at 1200°C

Ref: A. Misra, G. Ghosh, G.B. Olson, J. Phase Equilibria and Diff., vol. 25(6), 2004.

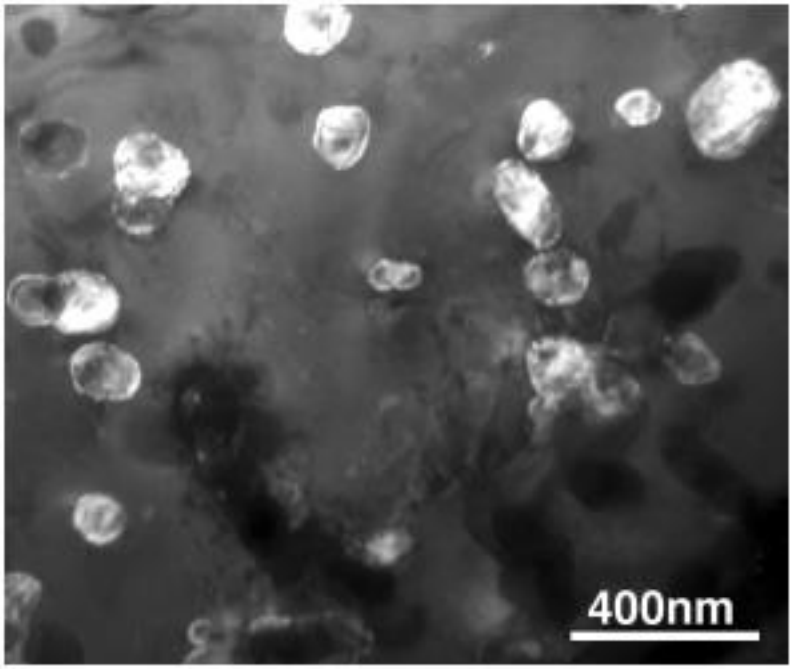
Dispersed Aluminides

DF-TEM Images

Heusler (Pd_2HfAl) precipitates in a **bcc Nb-based** matrix

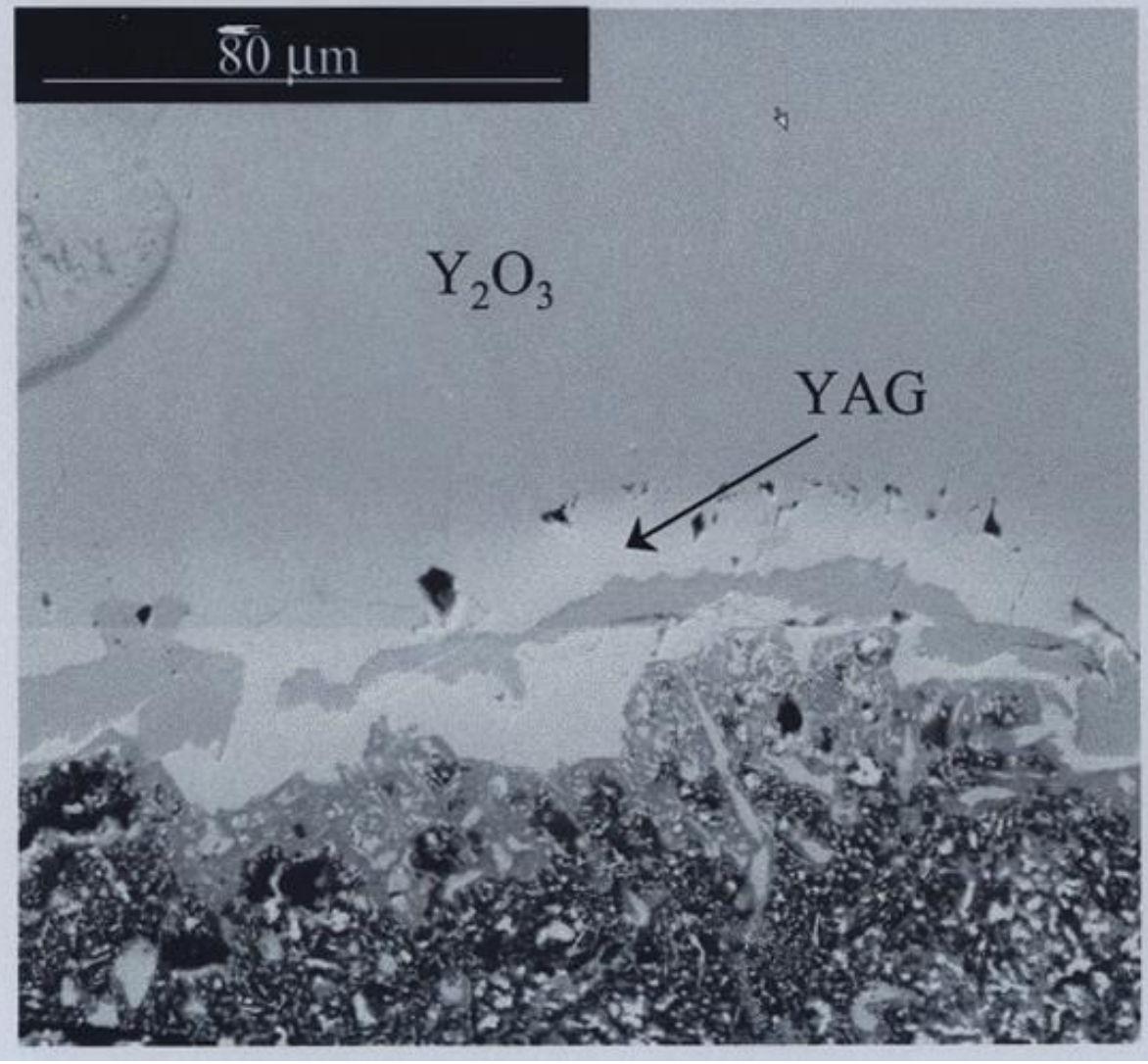


PdAl precipitates in a **bcc Nb-based** matrix

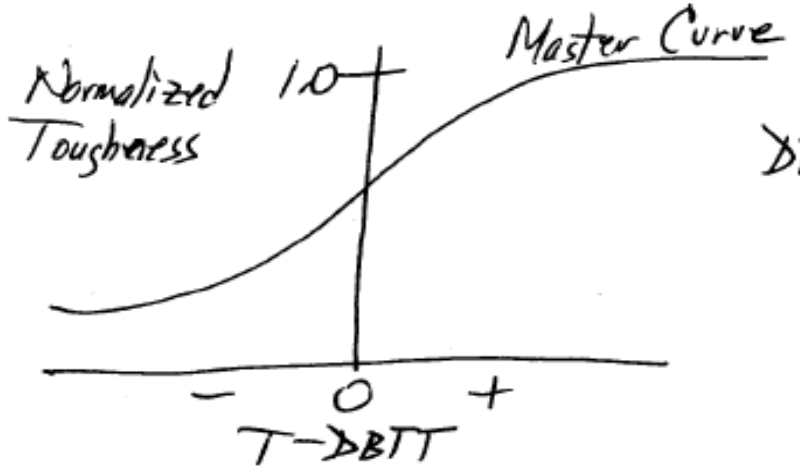


Ref: G. Ghosh, Northwestern Univ., 2002

Nb(Ti,Cr,Hf)-45PtYAl oxidized 1400°C 5 hours



Ductile vs Brittle

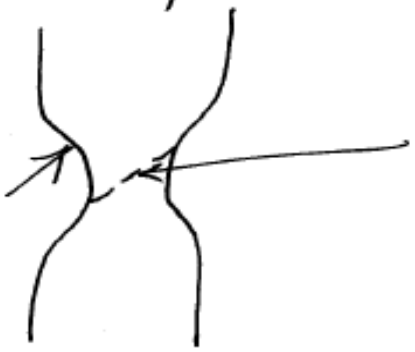


DBTT: D_{Grain} ↓, Ni ↑

Ductile Fracture

- primary voids
- microvoids + shear localization

Plastic Flow Stability



$\frac{d\sigma}{d\epsilon} \leq \sigma(true)$

Necking Instability (diffuse)

$\frac{d\sigma}{d\epsilon} \leq 0$

Shear Localization

Ductile Refractory Superalloy

	Room Temperature	2000°F
0.2% YS (ksi)	85.4	40.9
UTS (ksi)	102.8	47.3
% Elongation	24	11

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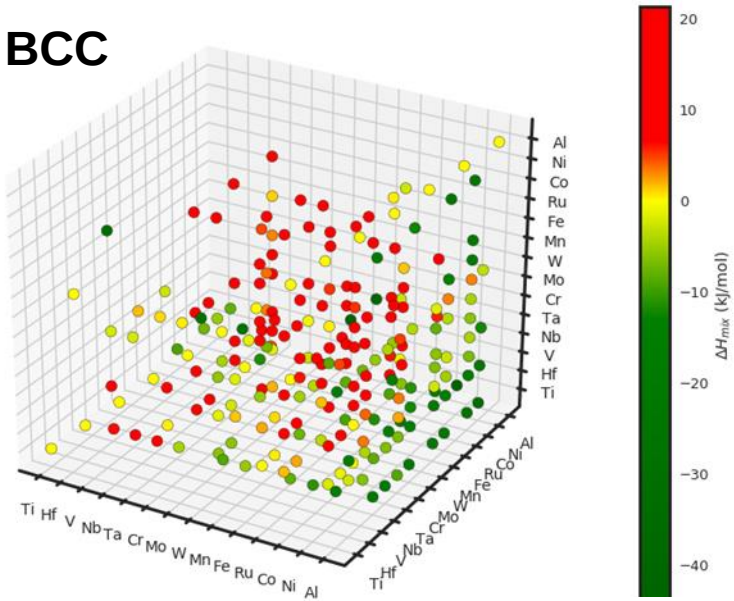
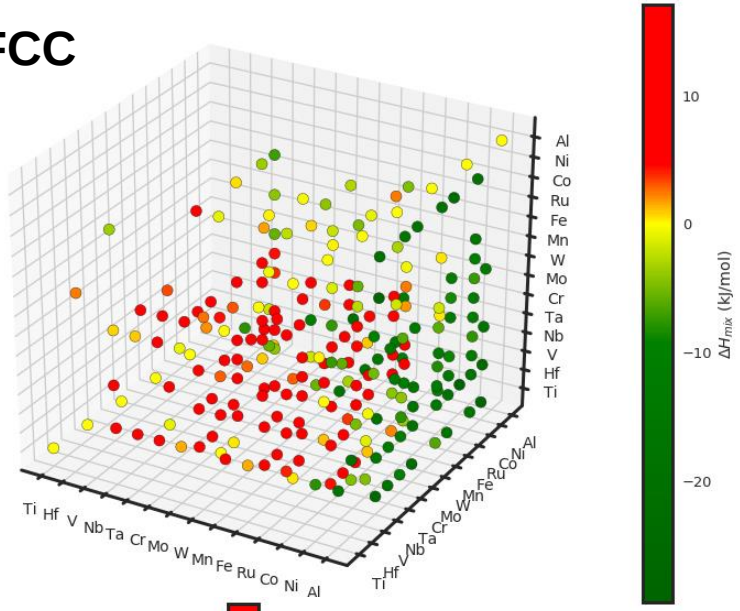
DFT Calculated Equiatomic Ternary Mixing Enthalpy

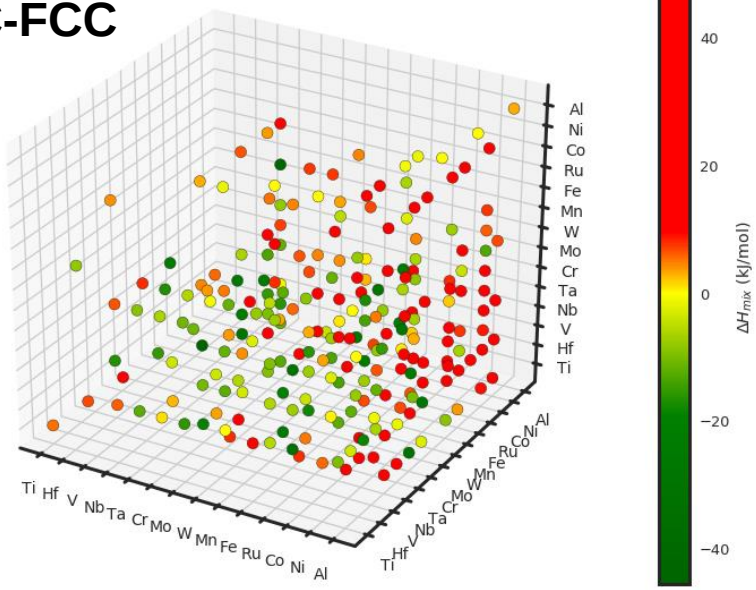
BCC



FCC



BCC-FCC



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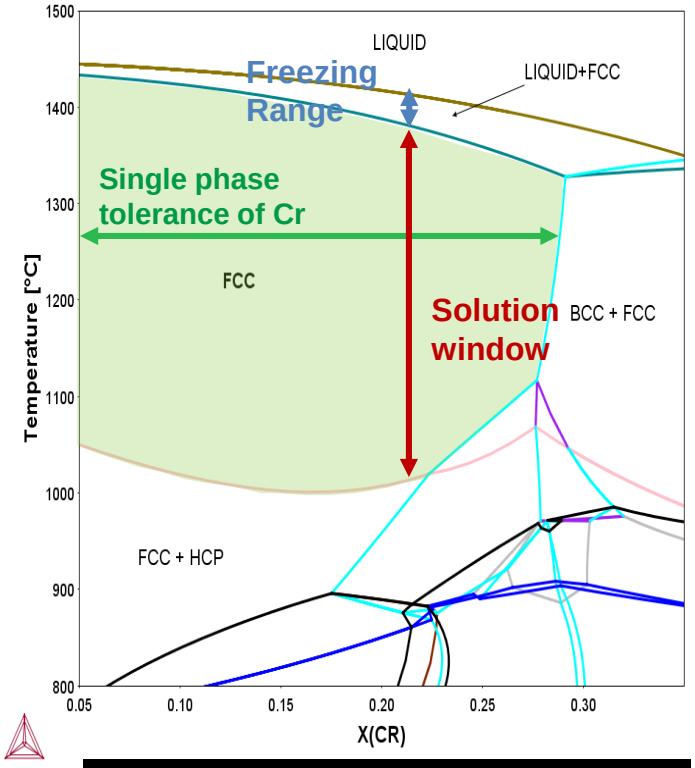
CALPHAD Design of FCC Corrosion Resistant HEAs:

-Enhanced solubility of Cr & Mo

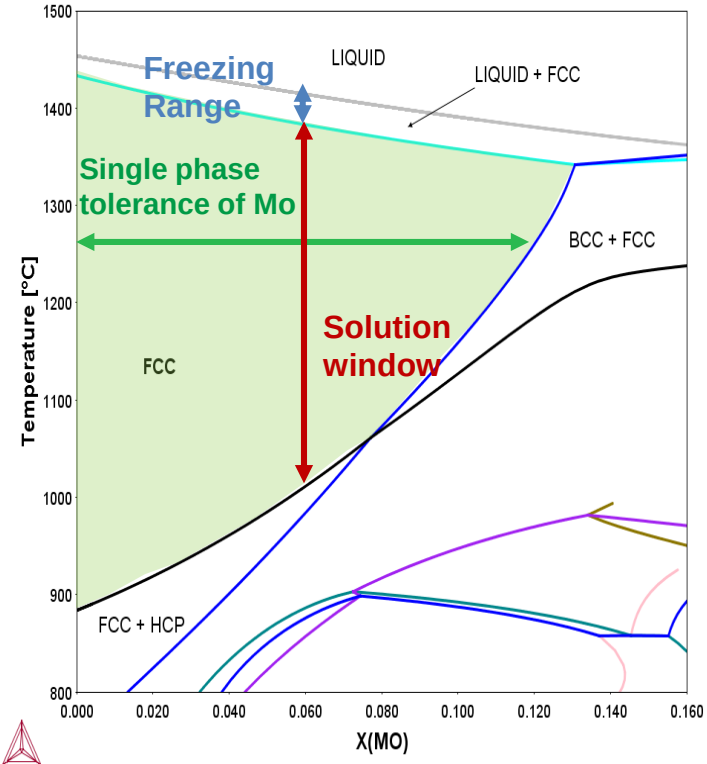
-Nonequiatomic optimal compositions

Cr for Ni:



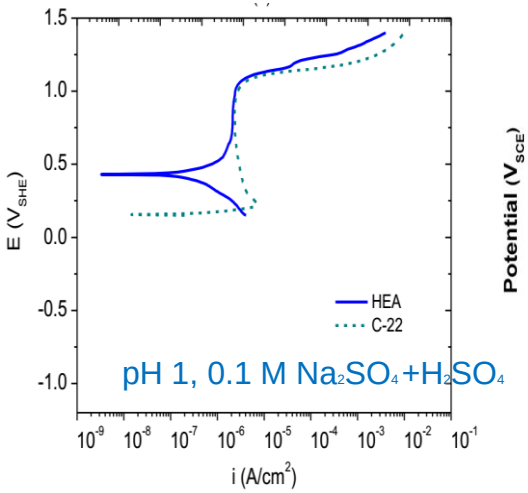
x in $Ni_{38-x}Cr_xFe_{20}Ru_{13}Mo_6W_2$

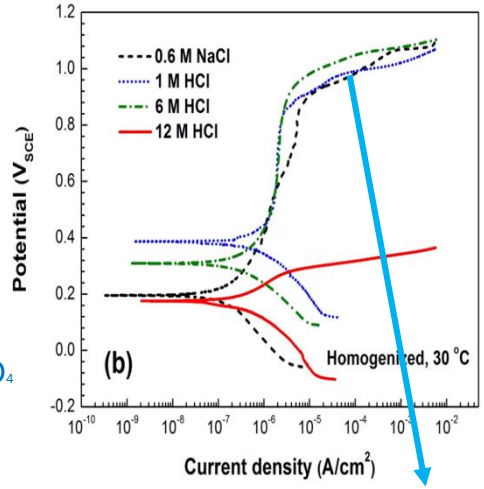
Mo for Ni:

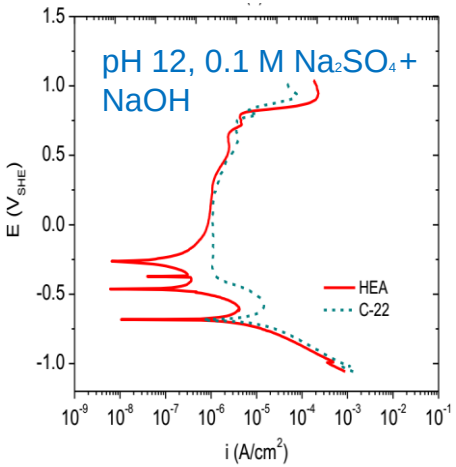


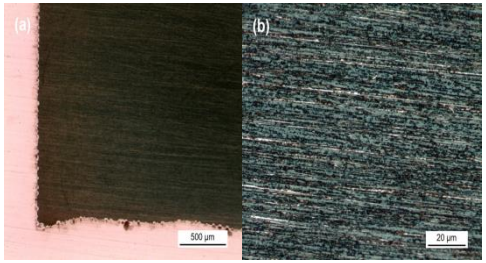
x in $Ni_{38-x}Cr_{21}Fe_{20}Ru_{13}Mo_{6-x}W_2$

Experimental Validation of $Ni_{38}Cr_{21}Fe_{20}Ru_{13}Mo_6W_2$ HEA









Excellent corrosion resistance in both aggressive sulfate and chloride environments

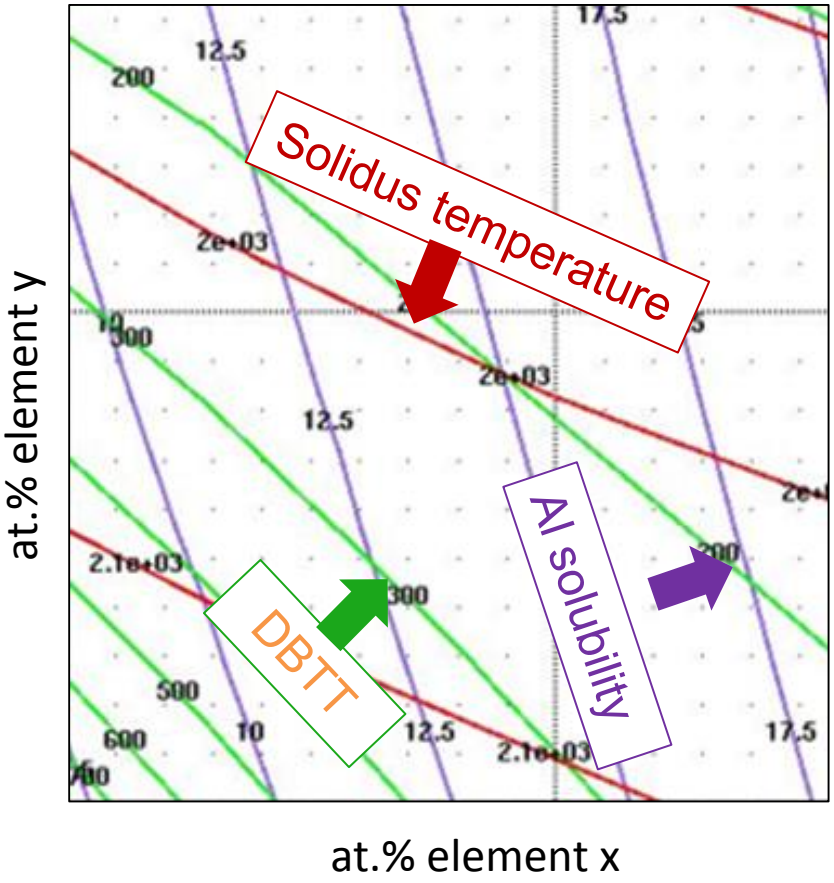
Uniform corrosion indicates transpassive dissolution instead of localized breakdown

QUESTEK® INNOVATIONS LLC

Refractory Alloys: CALPHAD-based Property Optimization

- Visualize property trade-offs as function of chemistry in an HEA
  - Maximize Al content to **maximize oxidation resistance**
  - Minimize DBTT to **maximize ductility**
  - Maximize $T_{solidus}$ to **maximize operating temperature**

- Contours of Al solubility at 1250°C, DBTT and solidus temperature, as function of Al content at fixed (x, y) ratios



Overview: QuesTek Innovations LLC

- Founded 1997 by Prof. Greg Olson, Ray Genellie, and Dr. Charlie Kuehmann

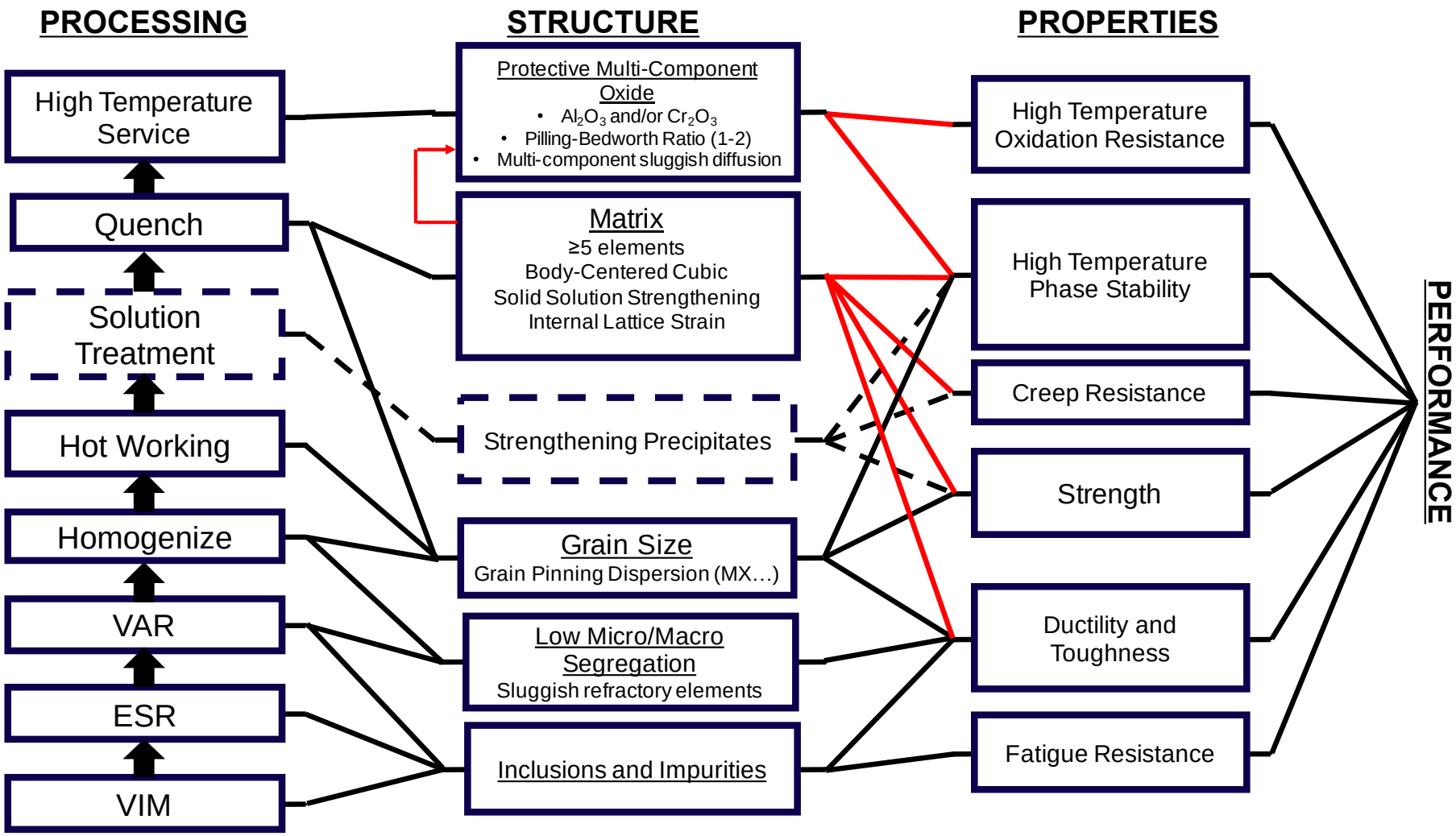
  -Northwestern University “spin-off”
- 30 full-time employees (16 PhDs)
- 7 member Board of Directors (4 National Academy of Engineering)
- Global leader in “integrated computational materials engineering” (ICME)
- Designing/deploying novel materials for government and industrial sectors (e.g., Energy, Aerospace, Automotive, Defense)
- Business model: Create IP and license to Producers / Processors / End-Users

QUESTEK® INNOVATIONS LLC

12	13	22	26	27	28	29	41	42	47	72	74
Mg	Al	Ti	Fe	Co	Ni	Cu	Nb	Mo	Ag	Hf	W
Magnesium	Aluminum	Titanium	Iron	Cobalt	Nickel	Copper	Niobium	Molybdenum	Silver	Hafnium	Tungsten

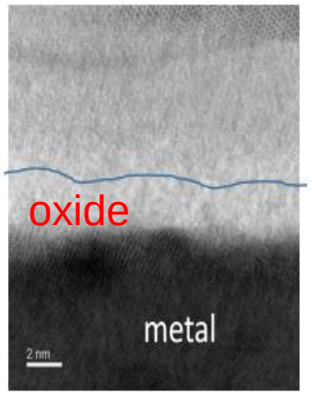
Backup Slides

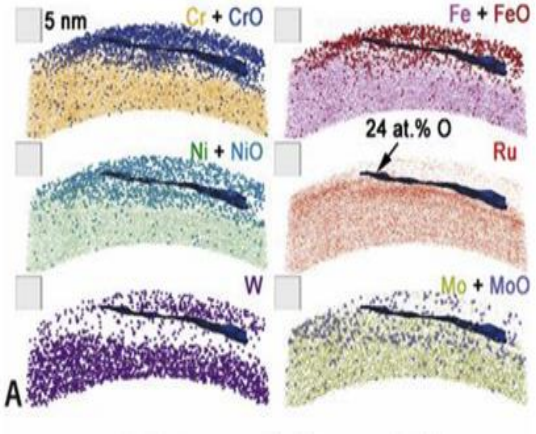
HEA turbine blade system chart

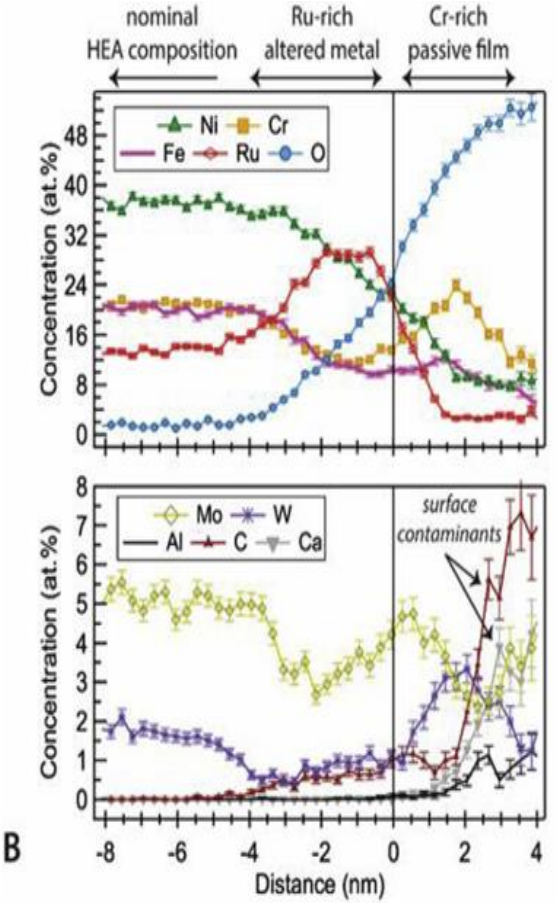


Experimental Validation of $Ni_{38}Cr_{21}Fe_{20}Ru_{13}Mo_6W_2$ HEA

A non-stoichiometric, compositionally complex oxide

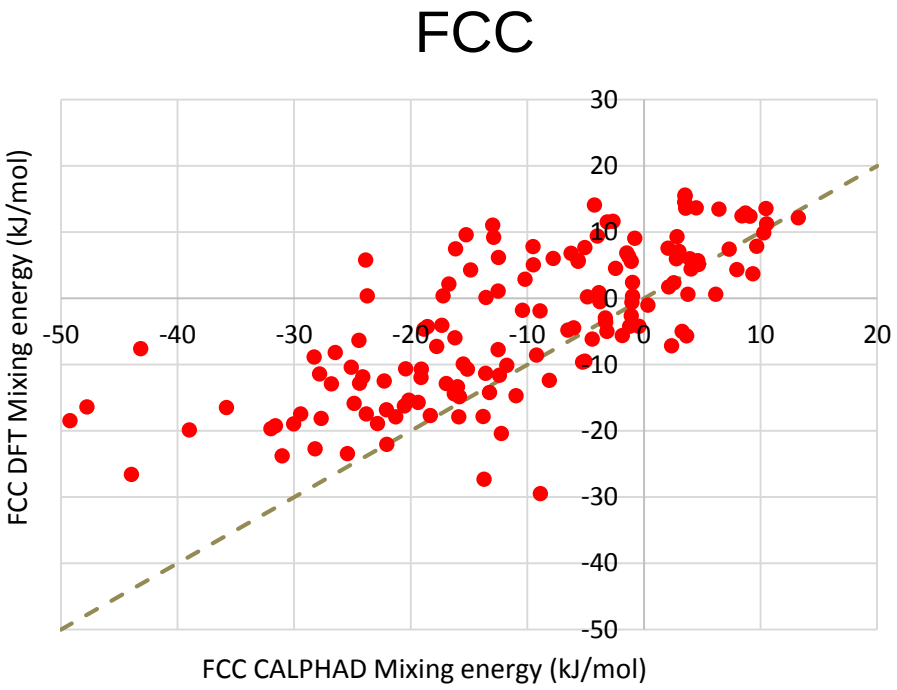


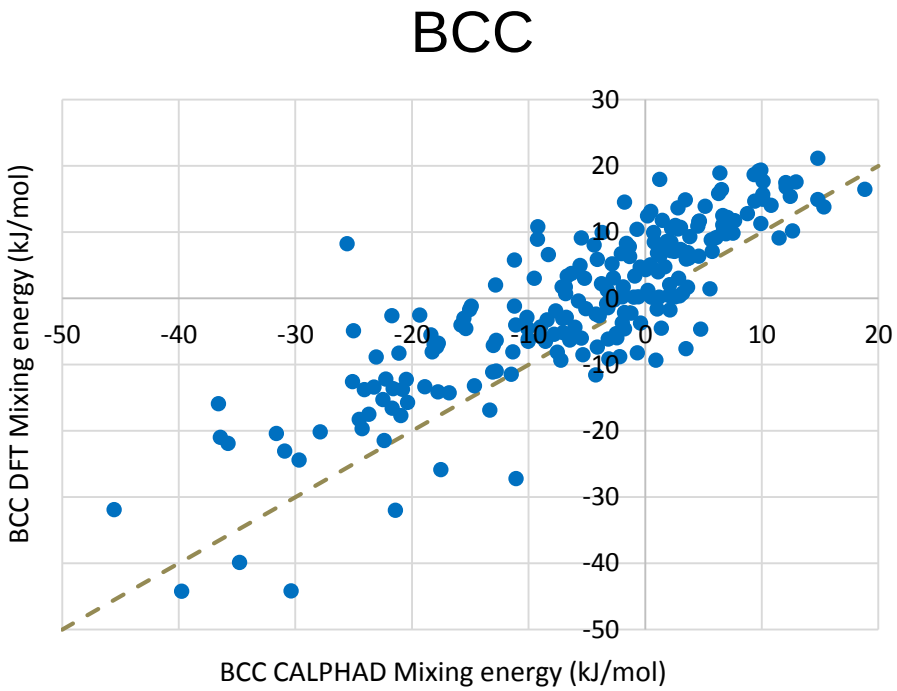




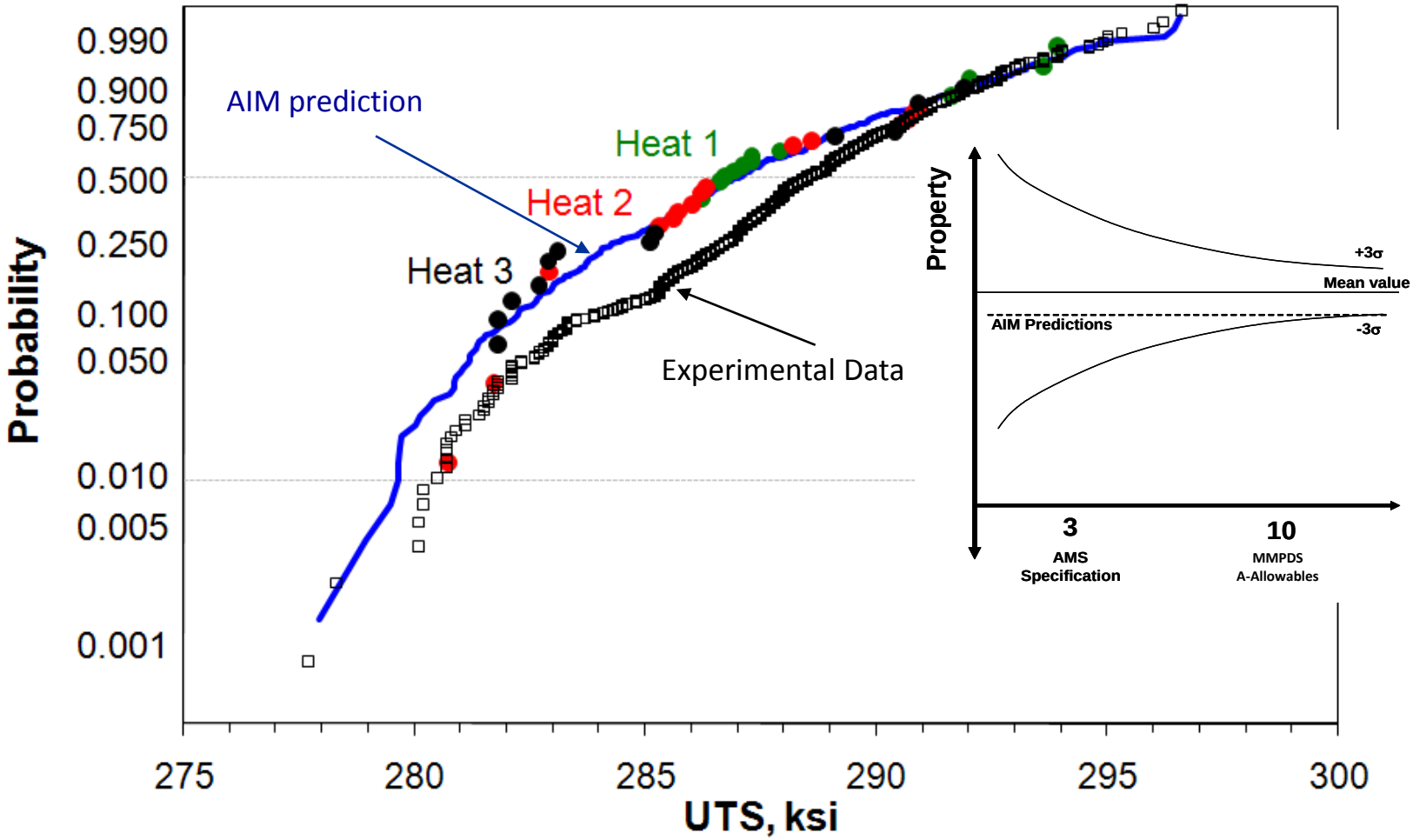
Quiambao, Kathleen F., et al. "Passivation of a corrosion resistant high entropy alloy in non-oxidizing sulfate solutions." *Acta Materialia* 164 (2019): 362-376.

DFT vs CALPHAD





S53 AIM Analysis for UTS



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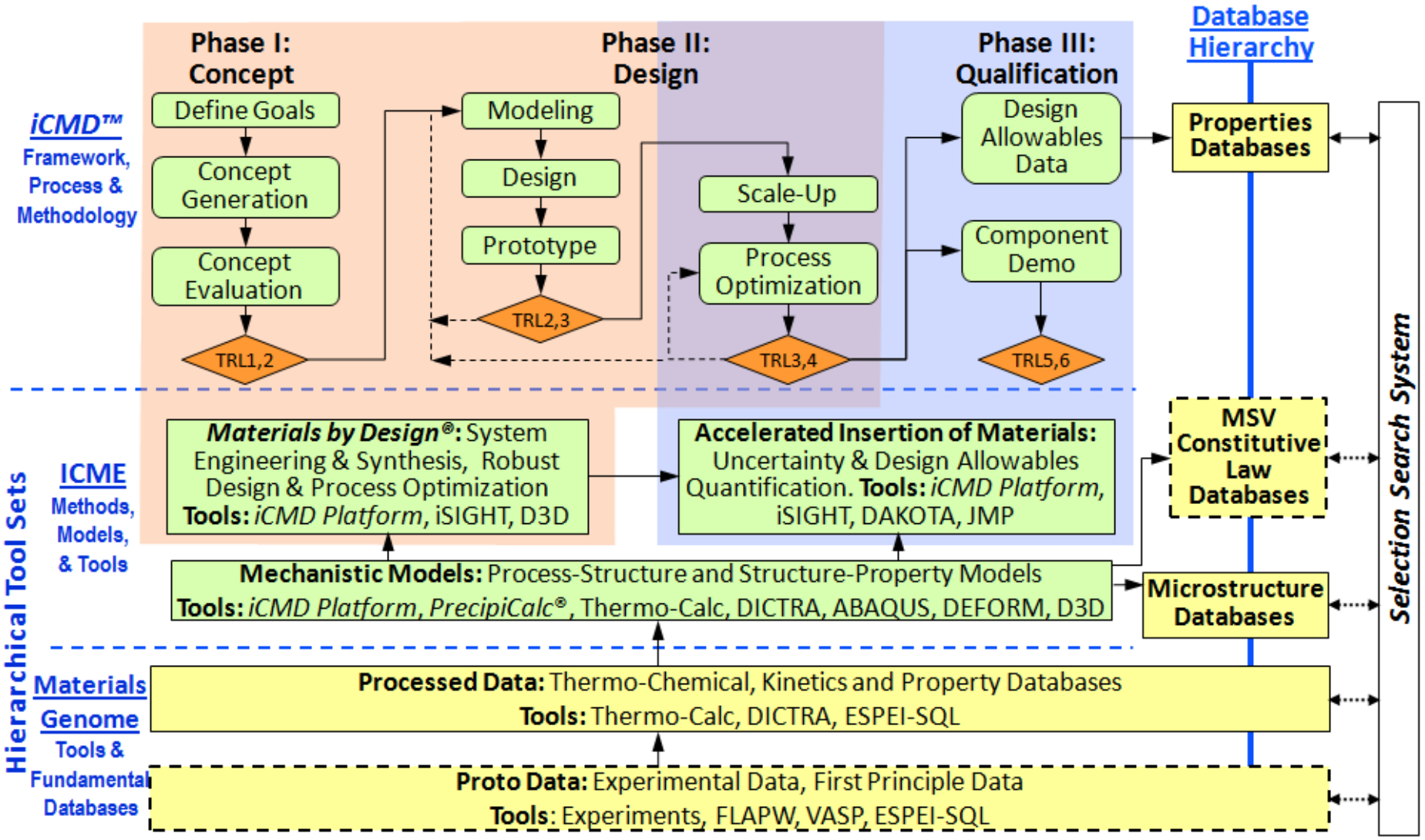

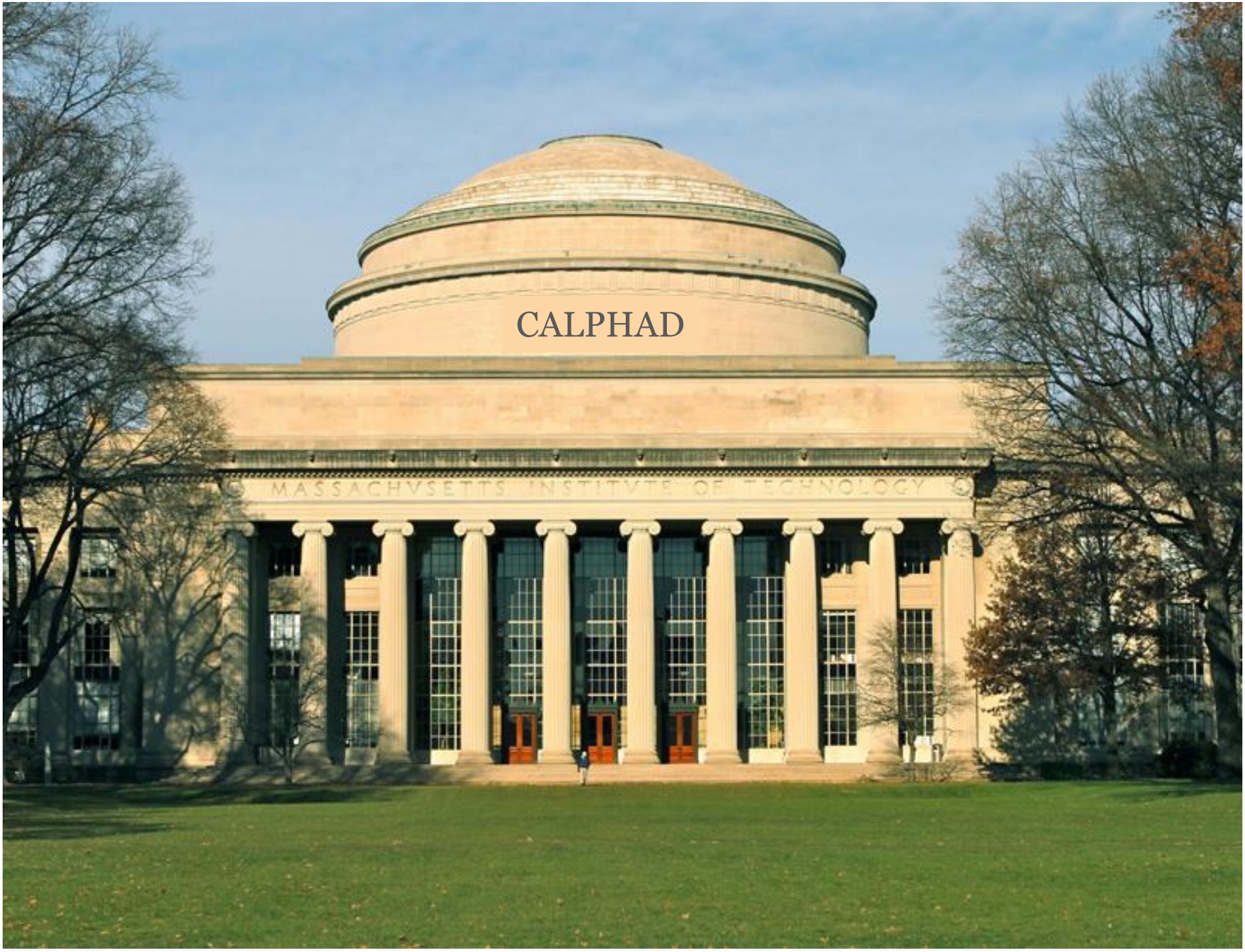
CALPHAD
MASSACHVSETTS INSTITVTE OF TECHNOLOGY