

Computational Materials Design: Affordable Change



G.B. Olson
ThermoCalc Professor of the Practice
MIT
& QuesTek Innovations LLC



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

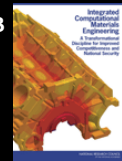
QUESTEK®
INNOVATIONS LLC

Materials Genome Timeline

2004 NMAB
Accelerating
Technology
Transition



2008 NMAB
ICME

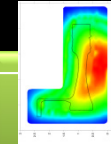


2011
OSTP

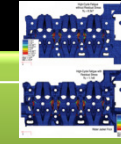


Integrated Computational Materials Engineering

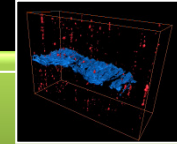
2001 DARPA
AIM



2003 Ford
VAC



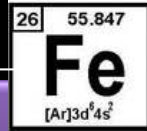
2005 ONR/DARPA
D3D



Concurrent
Engineered
Systems

Computational Materials Design

1985
SRG
Systems
Approach



Ferrous Alloys

1989
NASAlloy



1997
Ferrium C61™



Ni-base Alloys

2000
Ferrium S53®



Refractories

2004
Ferrium C64™



SMAs
Al-base Alloys

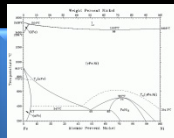
2007
Ferrium M54™



Cu-base Alloys

Alloys
Polymers
Ceramics
Composites

Materials
Genome



1956
Kaufman & Cohen



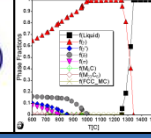
1973
CALPHAD



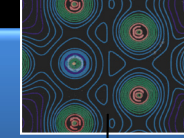
1979-84
Thermo-Calc
SGTE



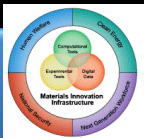
1990s
DICTRA
Pandat
Thermotech



PrecipiCalc®



2000s
DFT Integration



2011
Materials
Genome
Initiative

Gen I

Gen II

Gen III

1950

1970

1980

1990

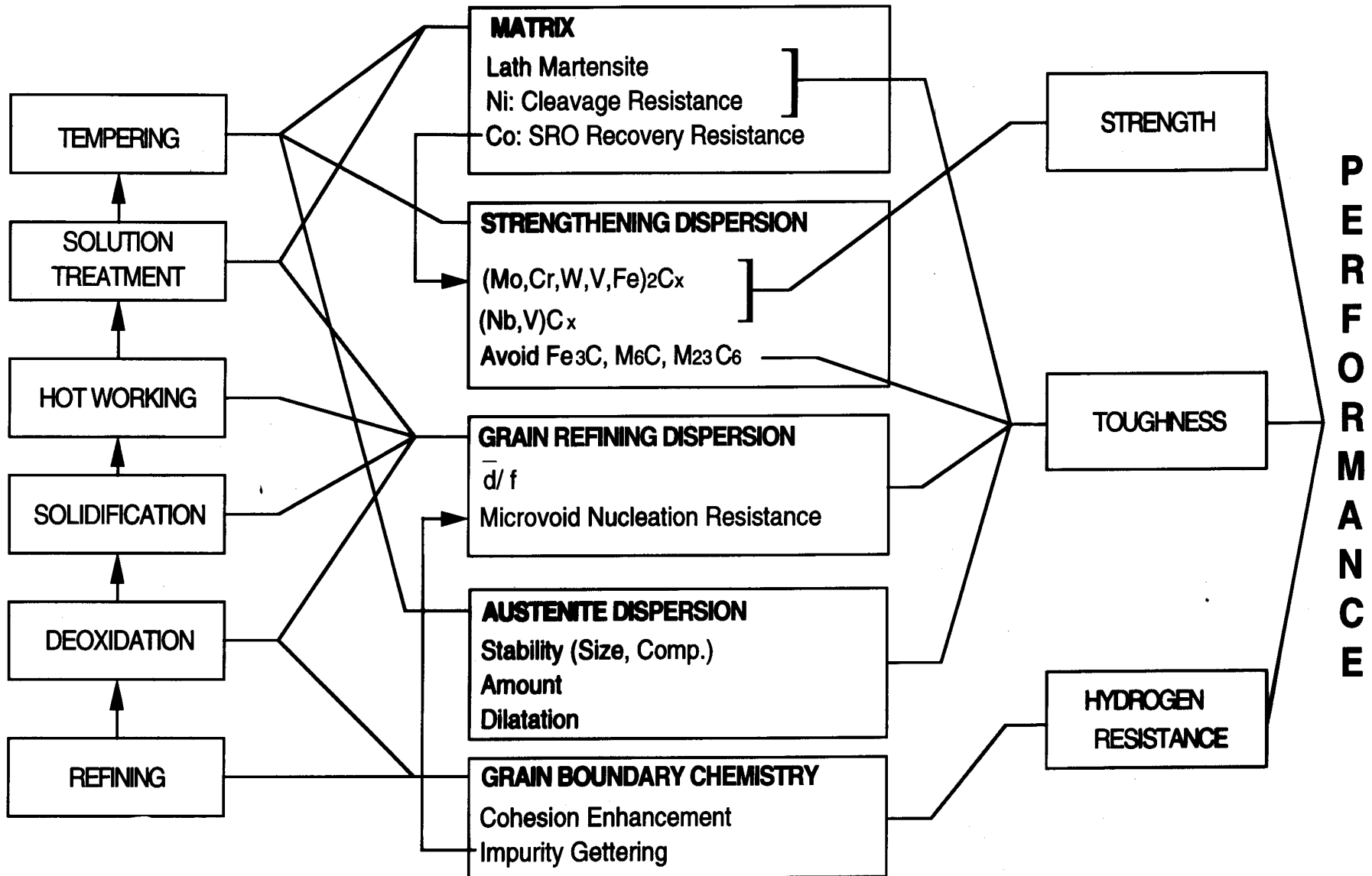
2000

2010

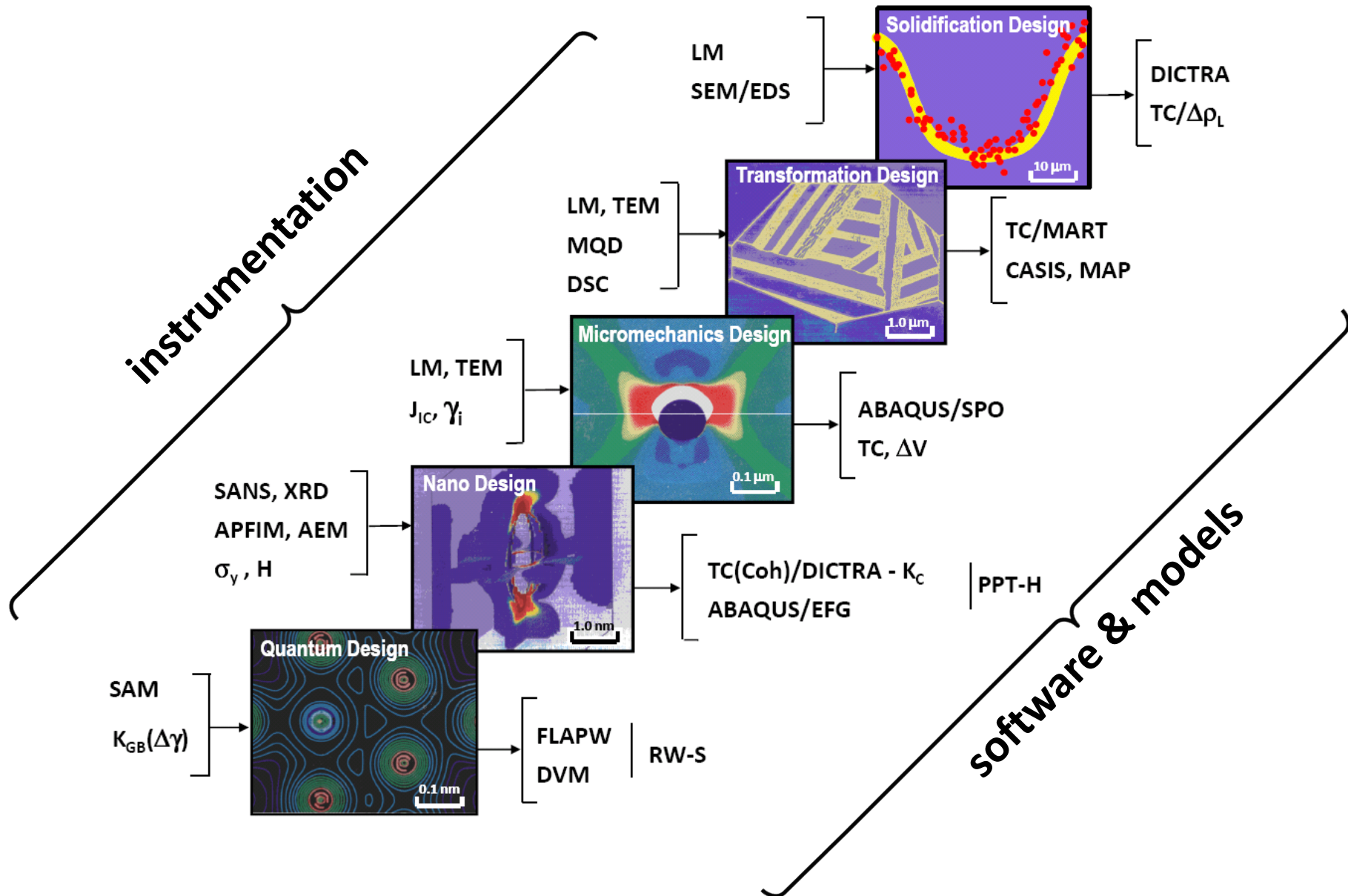
PROCESSING

STRUCTURE

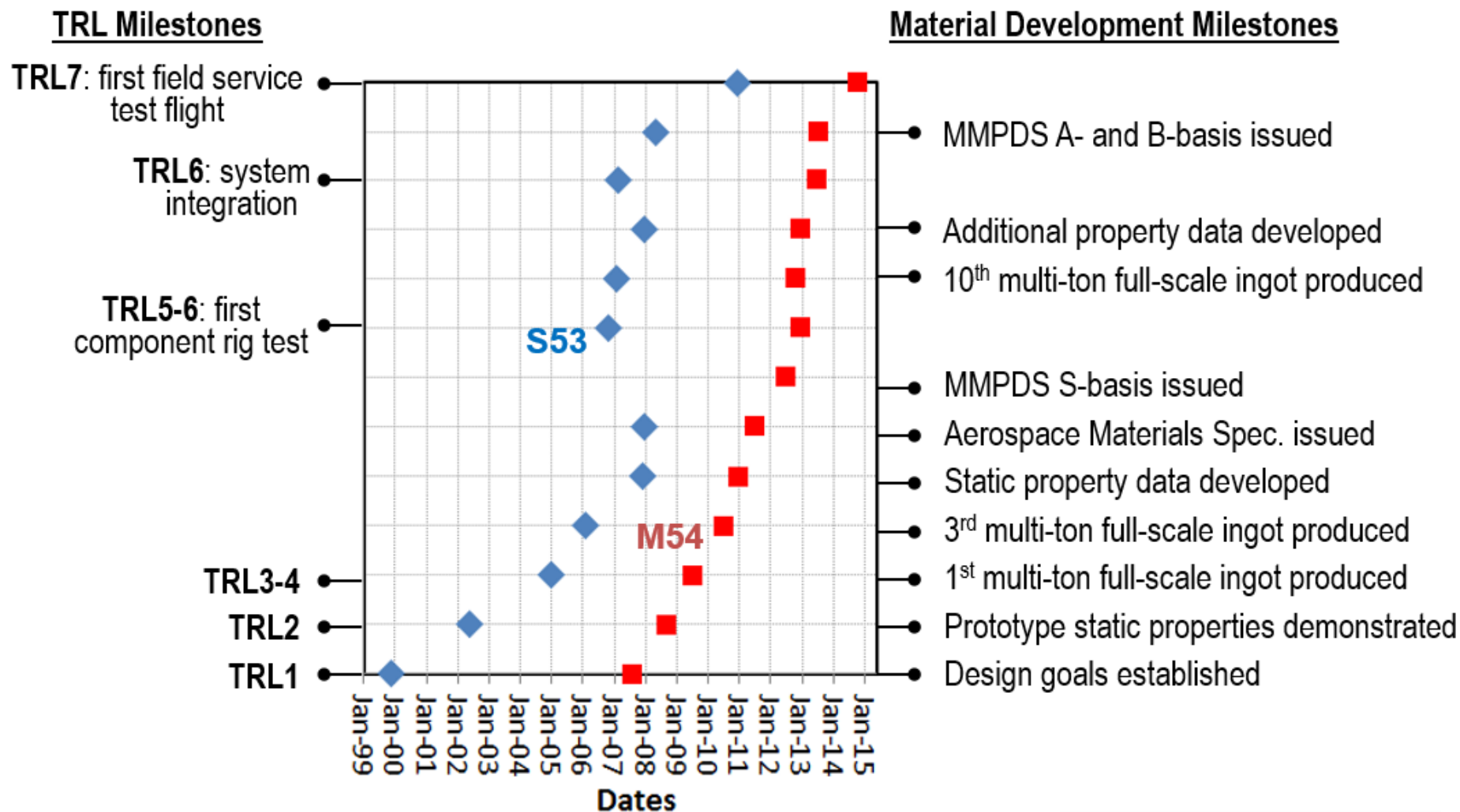
PROPERTIES



Hierarchy of Design Models



Computational Materials Qualification Acceleration





Apple watch

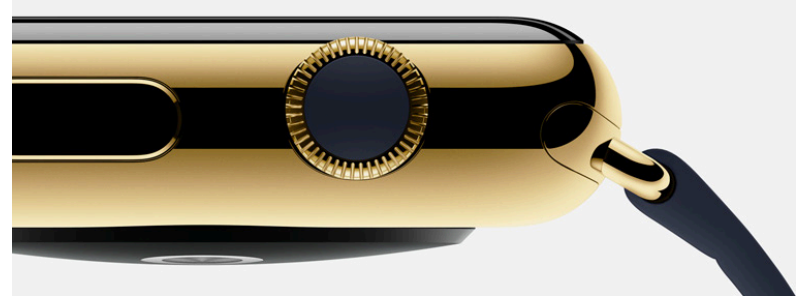
-Announced September 2014

Baseline: 316L Stainless Steel



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

High Strength 18K Gold



- 2X harder

Milanese Loop Alloy

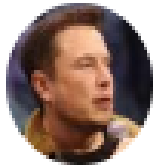


- Custom Magnetic Stainless Steel

Anodizable 7000 Aluminum



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



Elon Musk ✓

@elonmusk

Follow



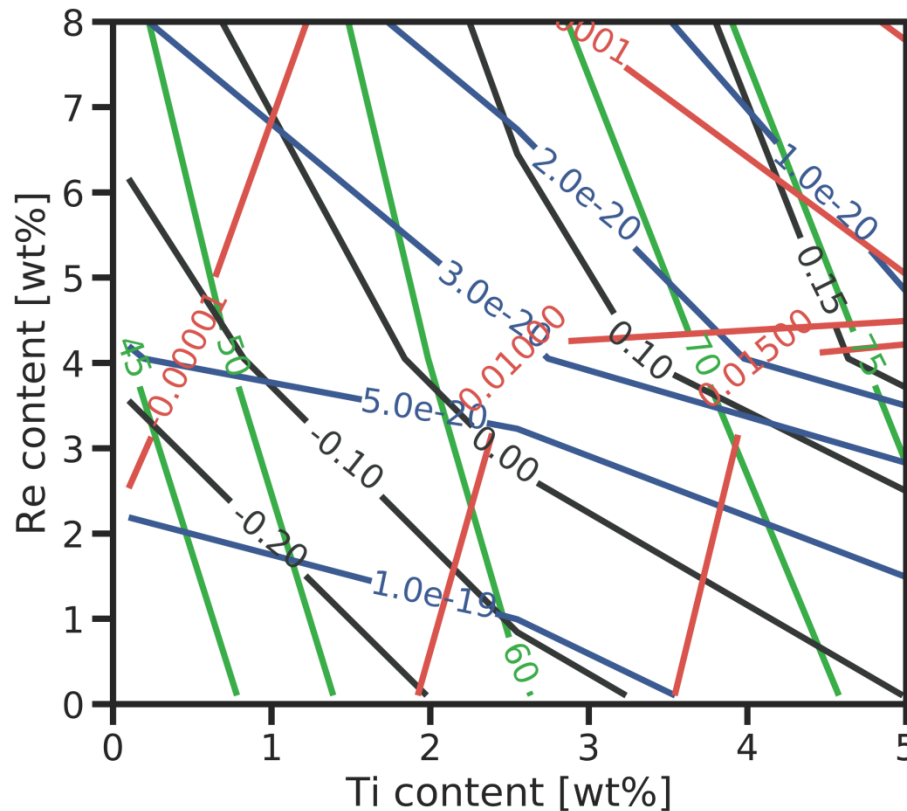
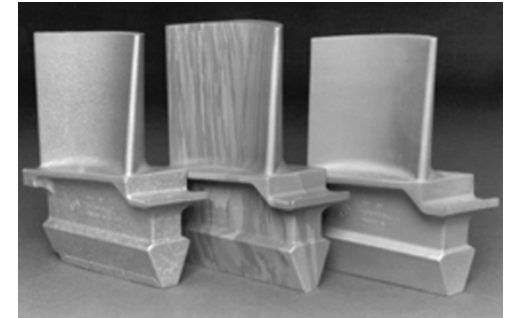
Replying to [@Robotbeat](#) [@Jon128123](#) and 8 others

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

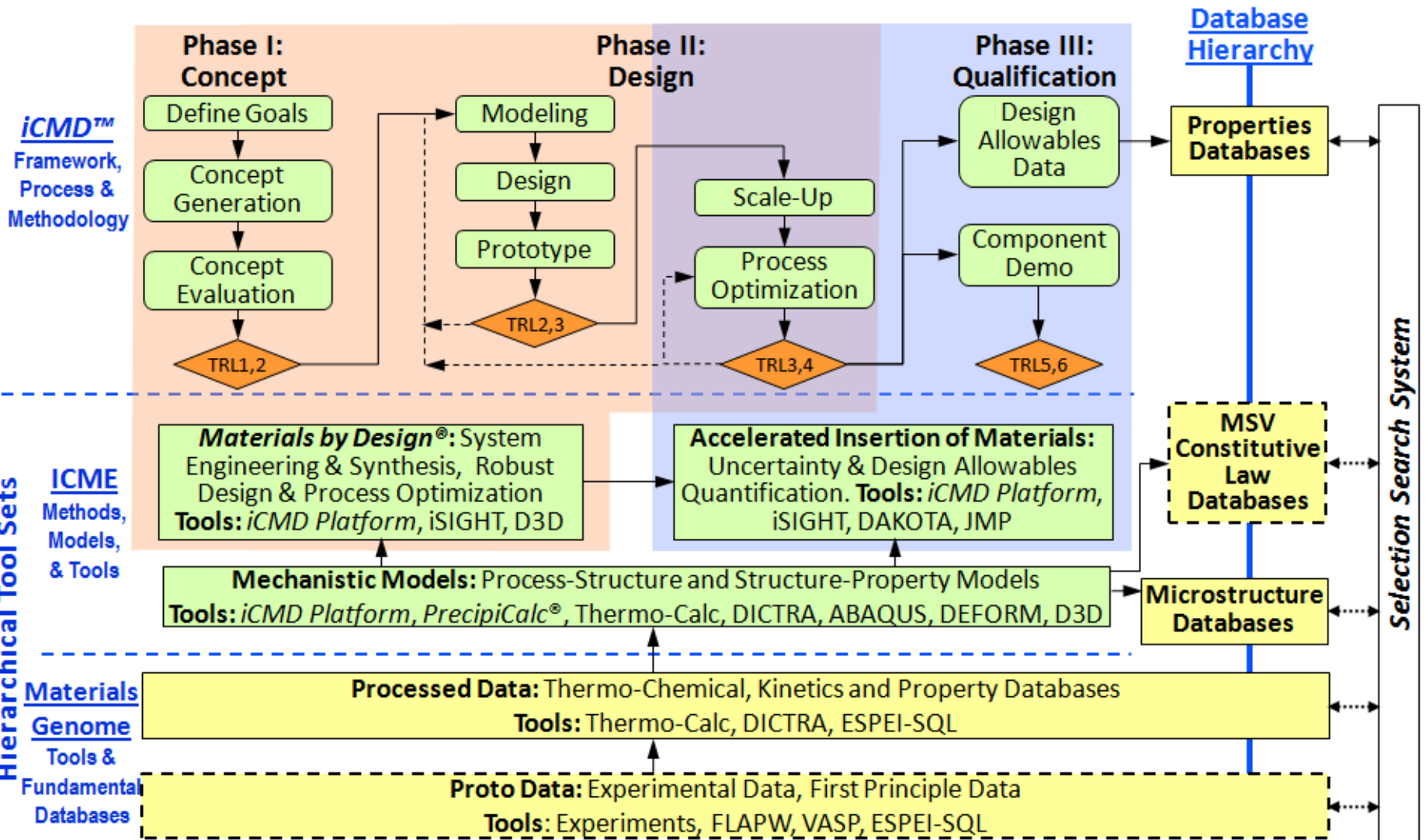
CALPHAD-based Design: Freckle-Resistant 1Re SX Ni Superalloy for IGT Blades

-Balancing liquid buoyancy and efficient Re partitioning for creep performance



Siemens SGT5-8000H 375MW Gas Turbine

Center for Hierarchical Materials Design



Backup Slides

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.

High-Entropy Alloys at QuesTek

- **DOE**

- 2015-2018** – “Exploration of High-Entropy Alloy (HEAs) for Turbine Applications”
 - Phase I and Phase II SBIR (DE-SC0013220)

- 2016-2020** – WastePD EFRC (Gerald Frankel PI)
 - Nuclear waste corrosion focus (waste form and canister)



- **DOD**

- 2016** – “An Integrated Computational Materials Engineering (ICME) Tool for the Streamlined Development of High-Entropy Alloys for Advanced Propulsion Systems”
 - Phase I STTR with University of Tennessee, Knoxville (N68335-17-C-0618)



- 2018-2021** – “HEA Binder Material Design in Enhanced Tooling for Friction Welding Technology”
 - Phase I and Phase II with University of North Texas



- 2019** – “Mechanistically Enhanced Machine Learning for Materials Design and Process Optimization”
 - Phase I STTR with Texas A&M University (N68335-19-C-0400)



- **NASA**

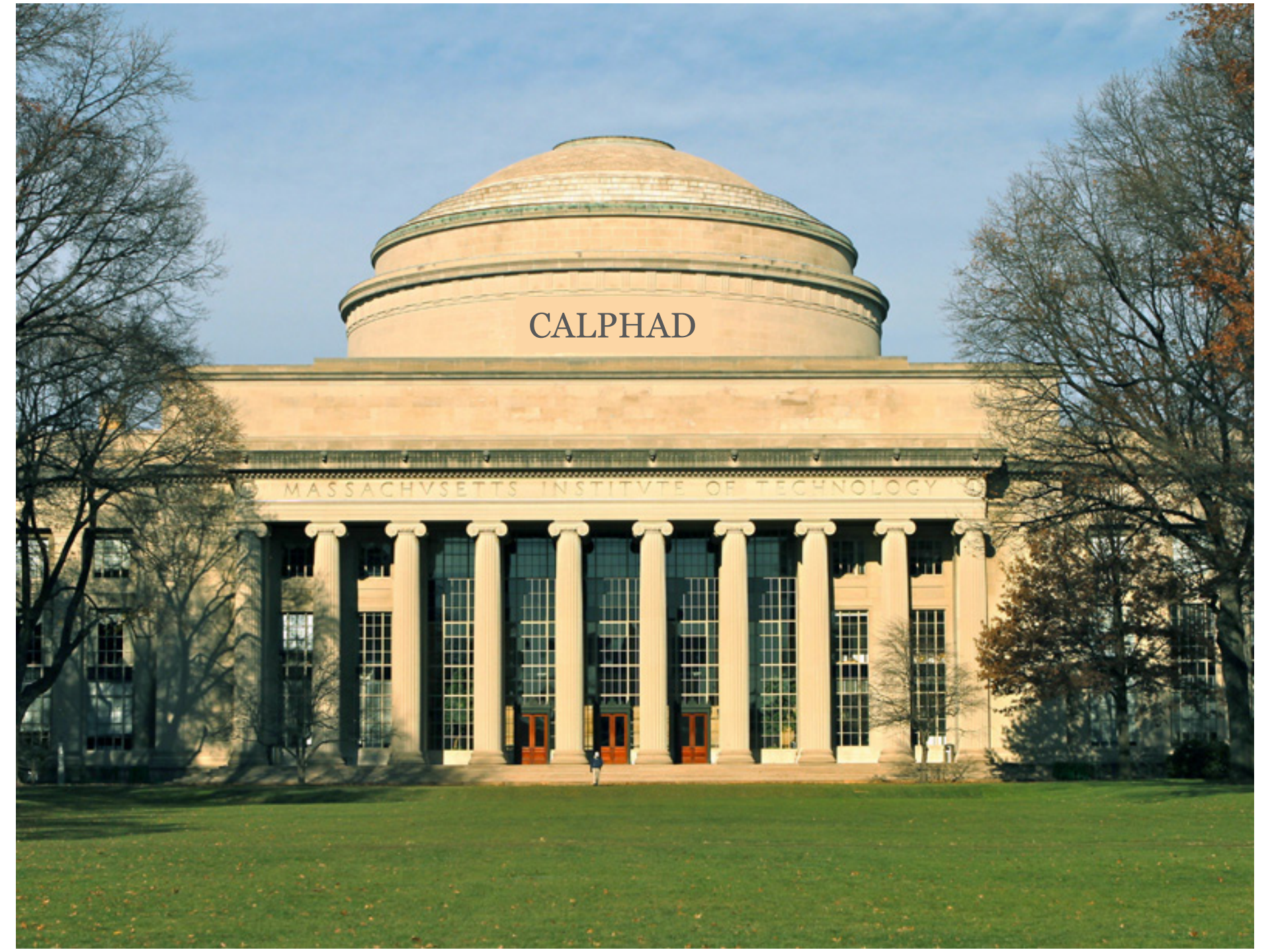
- 2019-2020** – “Tool Material Design for Friction Stir Welding of High Temperature Materials”
 - Phase I SBIR with University of North Texas



- **Commercial Collaboration: H.C. Starck**

- 2019-** – “Demonstration of Production and Thermomechanical Processing of Refractory CCAs”



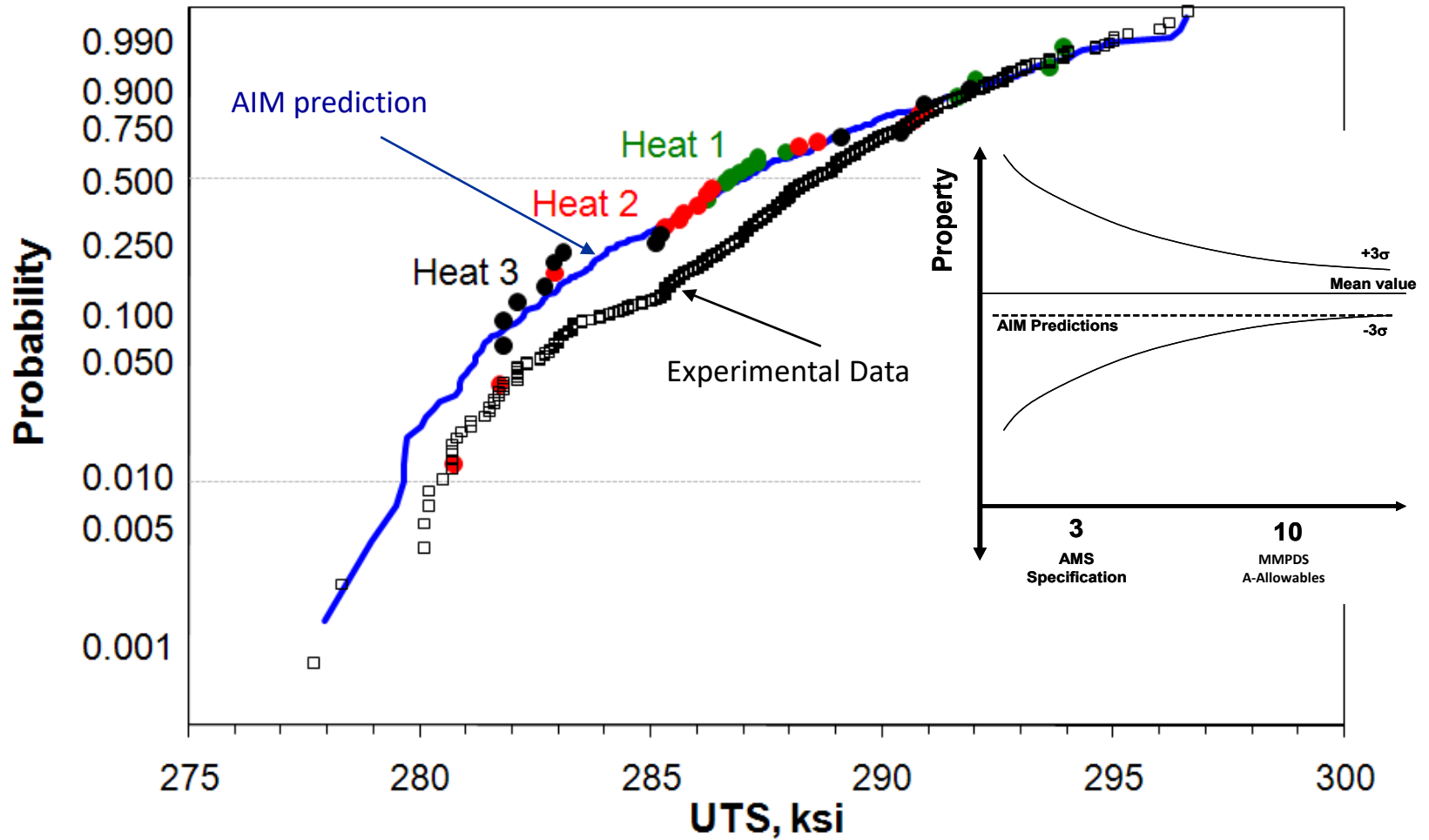
A photograph of the Massachusetts Institute of Technology (MIT) dome building. The building is a large, classical-style structure with a prominent dome. The facade features a row of columns and a pediment with the inscription "MASSACHUSETTS INSTITUTE OF TECHNOLOGY". The word "CALPHAD" is overlaid in a serif font on the dome. The building is surrounded by trees and a green lawn.

CALPHAD

MASSACHUSETTS INSTITUTE OF TECHNOLOGY



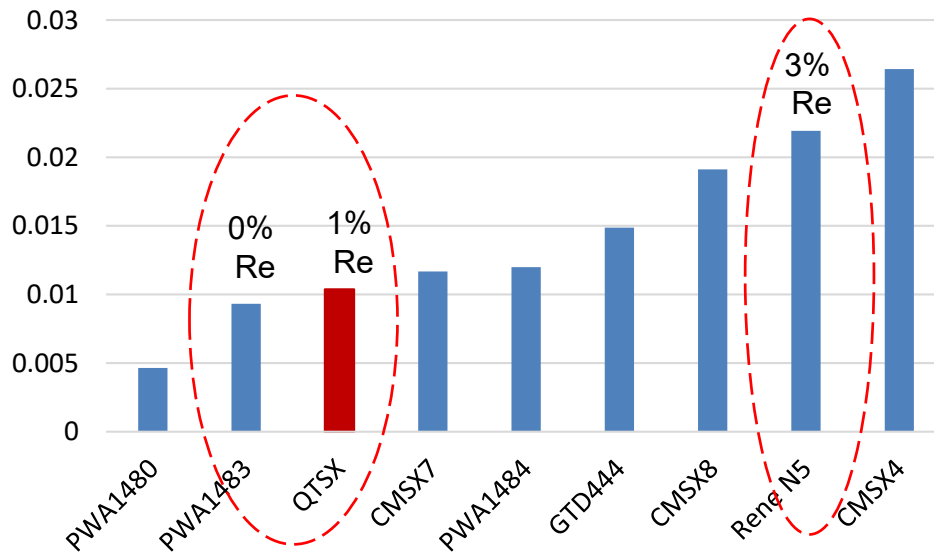
S53 AIM Analysis for UTS



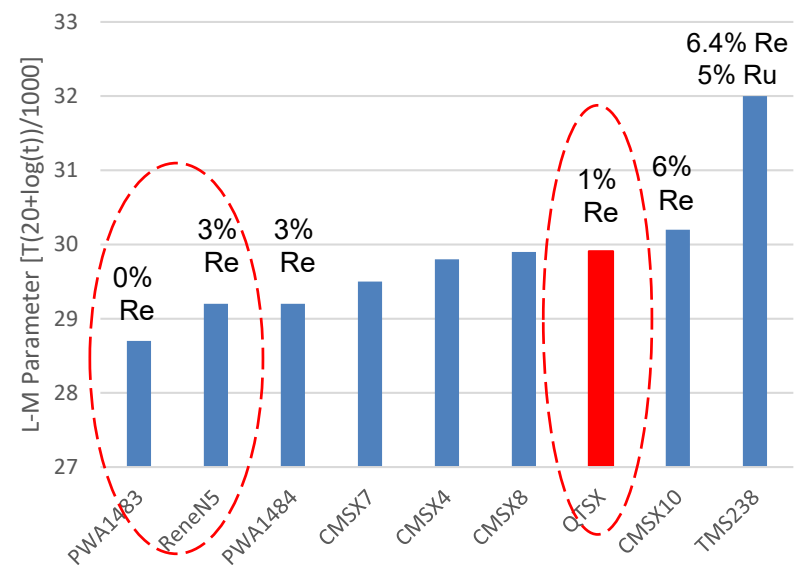
QTSX 1Re IGT SX Ni Superalloy

-Processability & Performance

Liquid density difference at 20% solidification

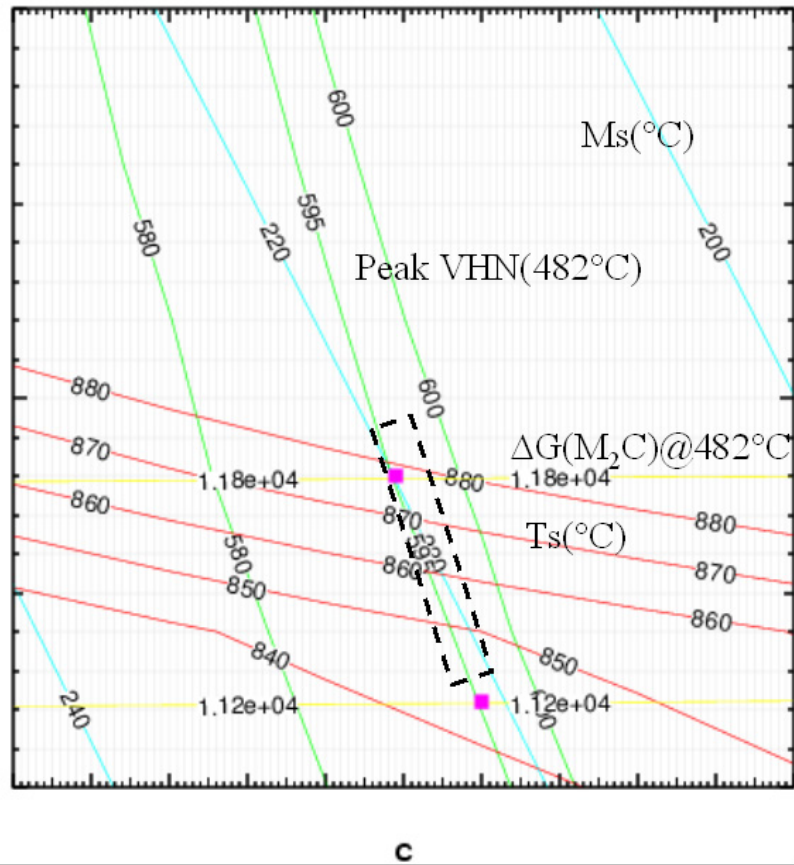


L-M Parameter at 150MPa

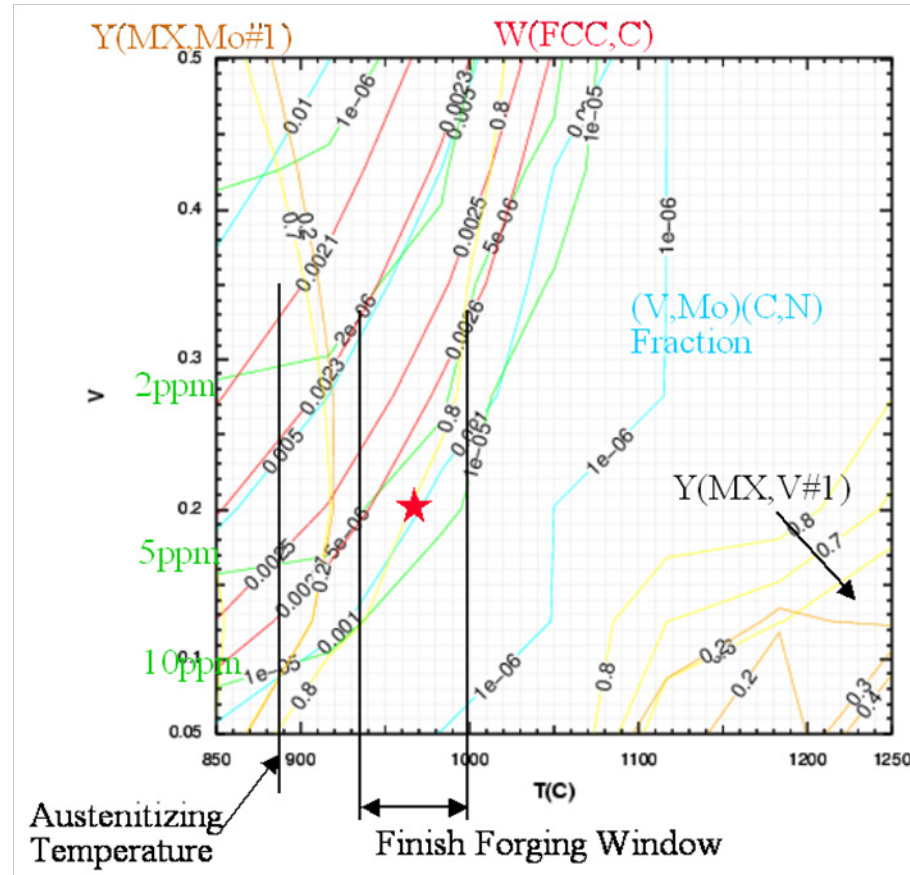


Example: Design Integration with CMD

Matrix + Strengthening
Dispersion Design



Grain Pinning Dispersion
Design



CyberSteels to Market

Ferrium C61

AMS6517

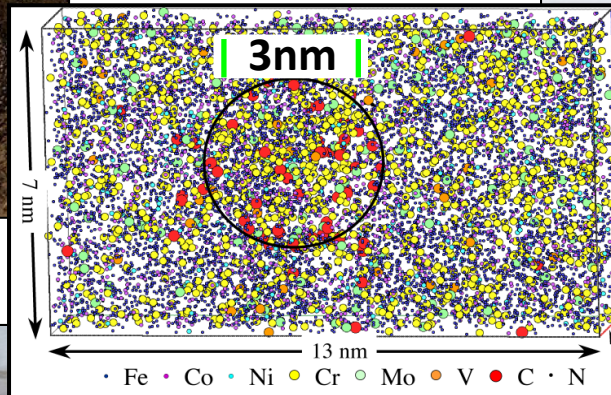


Ferrium S53 Stainless

AMS5922



A10



T45



Ferrium C64

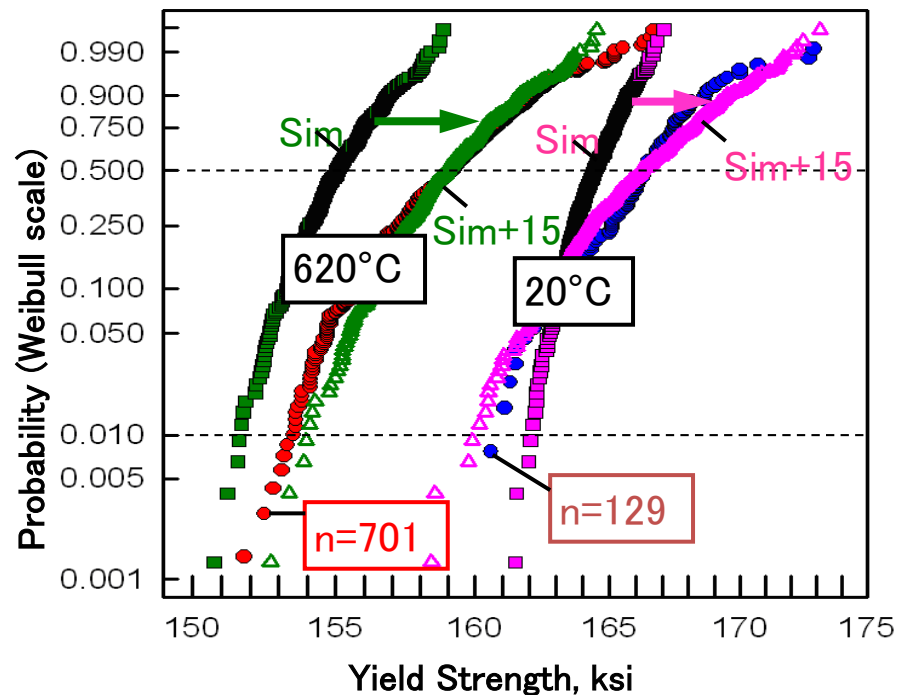
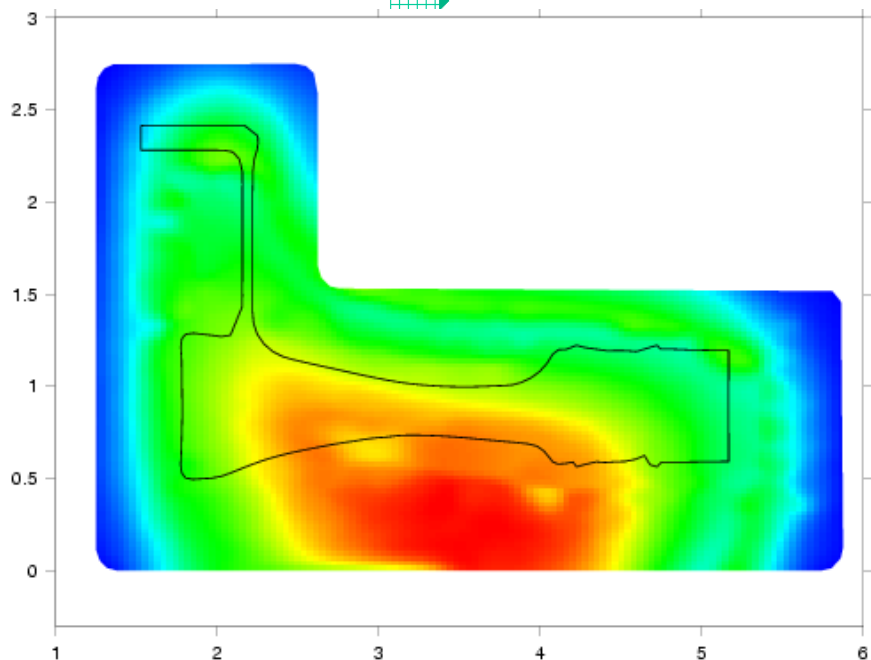
AMS6509

Ferrium M54

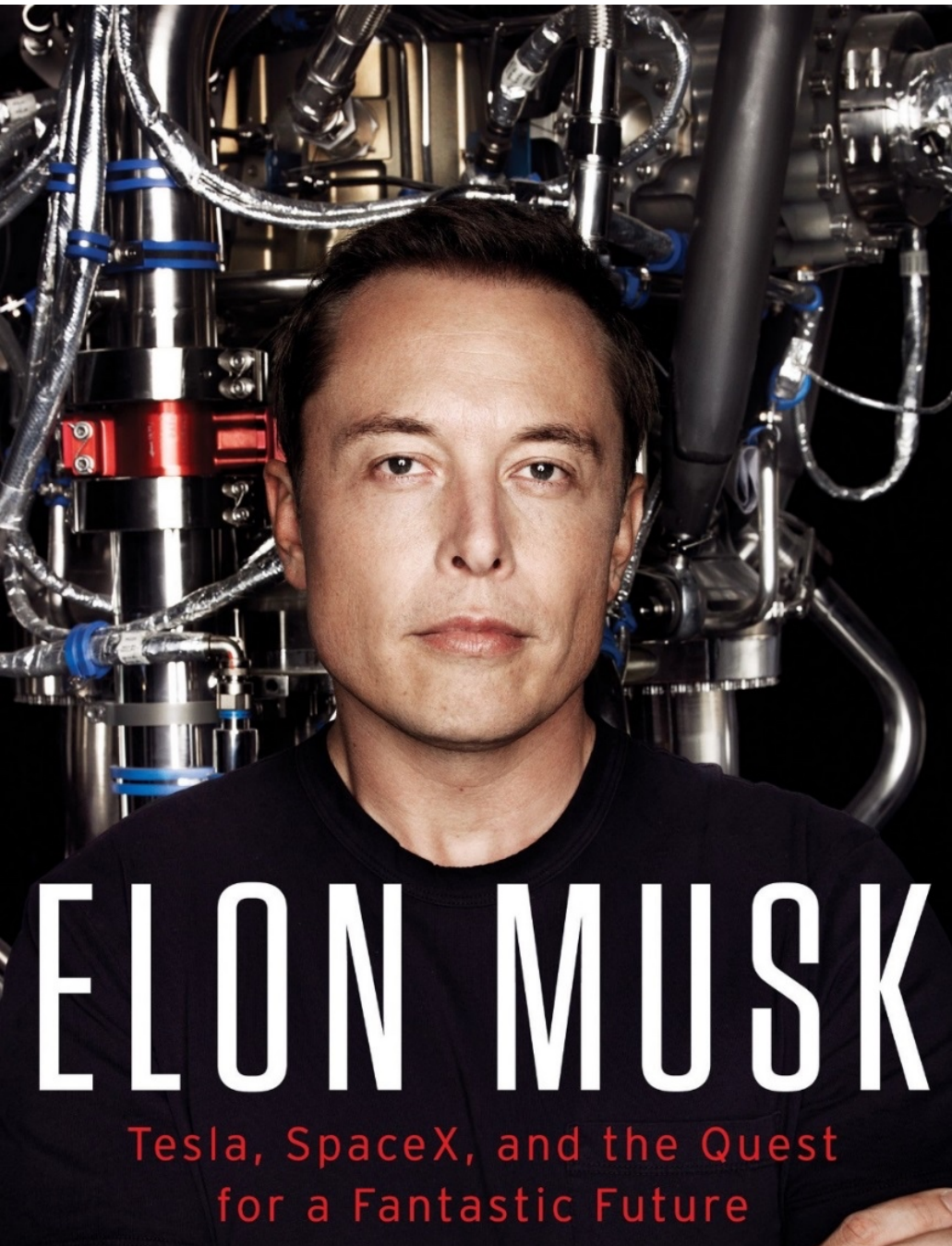
AMS6516



AIM
Accelerated Insertion of Materials

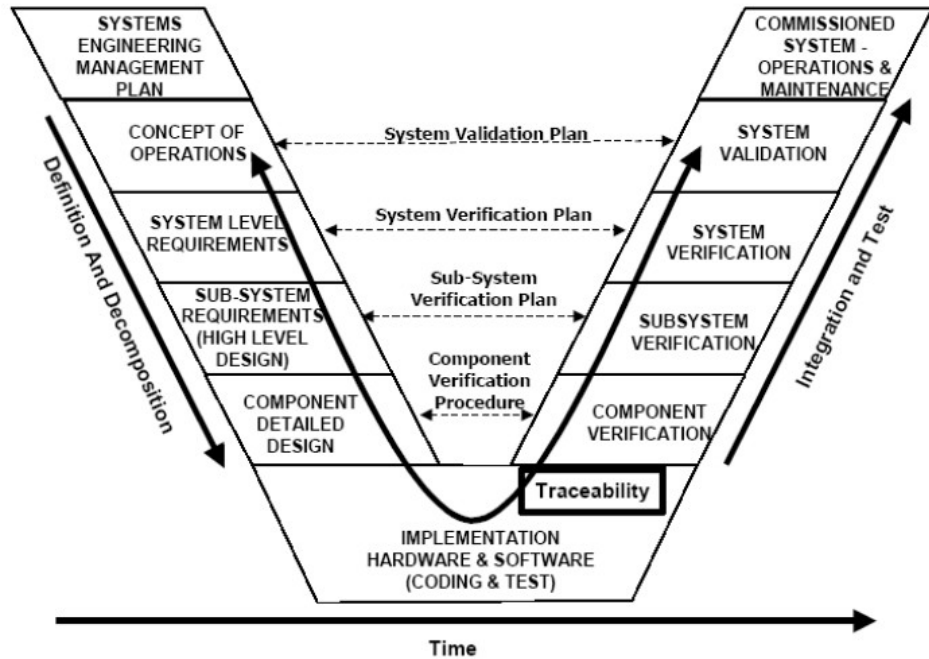


MGI: From Ferrium Ridge to Silicon Valley

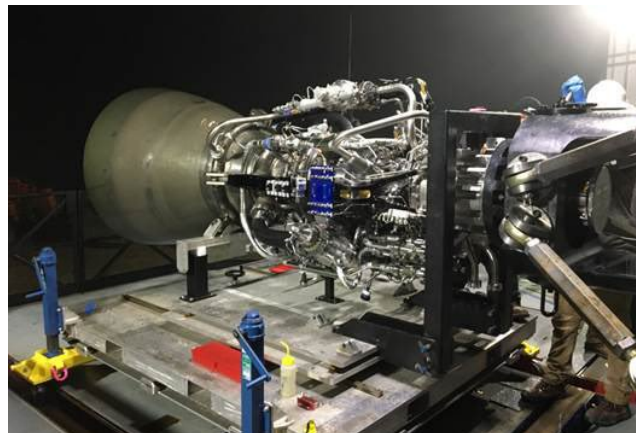
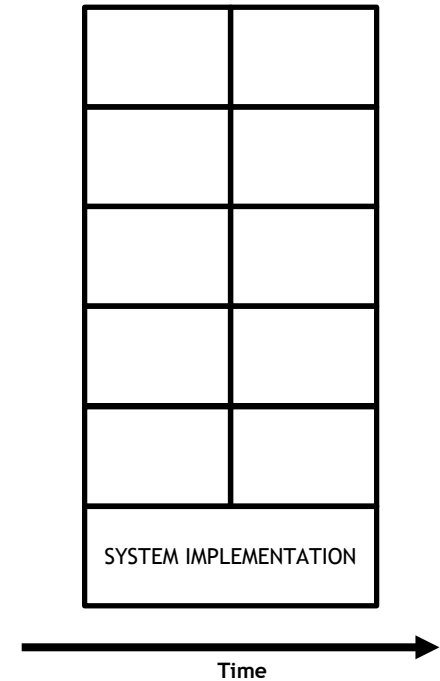


Manufacturing 5.0

Standard V-model for Systems Development Cycle



Total Concurrency



-After C. J. Kuehmann

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



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UNIVERSITY

QUESTek[®]
INNOVATIONS LLC



THE UNIVERSITY OF
CHICAGO

