NeoAlchemy:
Transmuting Data into New Materials

G.B. Olson

Northwestern University

&

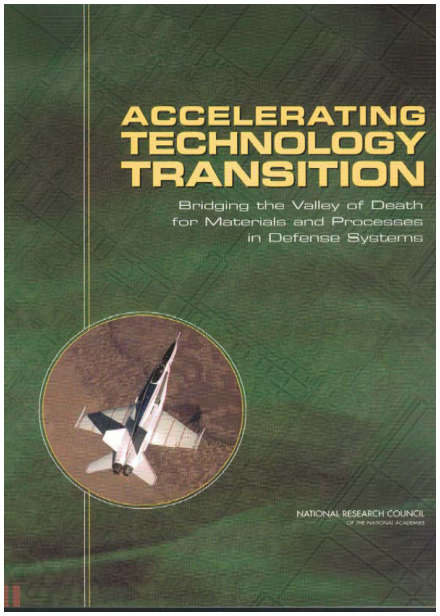
QuesTek Innovations LLC

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

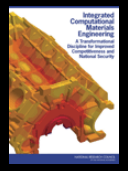
Material approval:	**November 2009**
Component approval:	**August 2010**
Component installation:	**November 2010**
First flight:	**December 2010**

QuesTek® INNOVATIONS LLC

Materials Genome Timeline

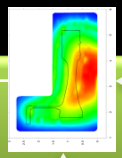
2004 NMAB Accelerating Technology Transition

2008 NMAB ICME



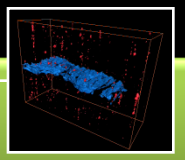
2011 OSTP

2001 DARPA AIM



2003 Ford VAC

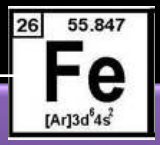
2005 DARPA/ONR D3D



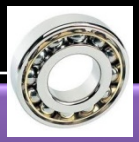
Concurrent Engineered Systems

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

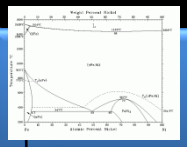
SMAs

Al-base Alloys

Cu-base Alloys

PrecipiCalc®

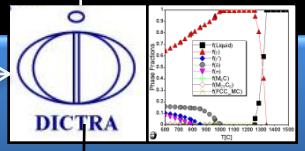
Materials Genome



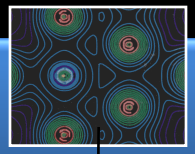
1956
Kaufman & Cohen

1973
CALPHAD

1979-84
Thermo-Calc
SGTE



1990s
DICTRA
Pandat
Thermotech



2000s
DFT Integration

2011
Materials
Genome
Initiative

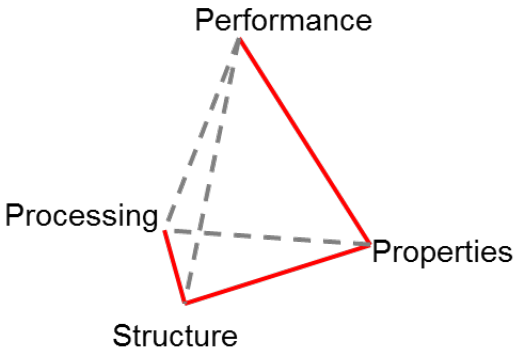
Gen I
1950
1970

Gen II
1980
1990
2000

Gen III
2010

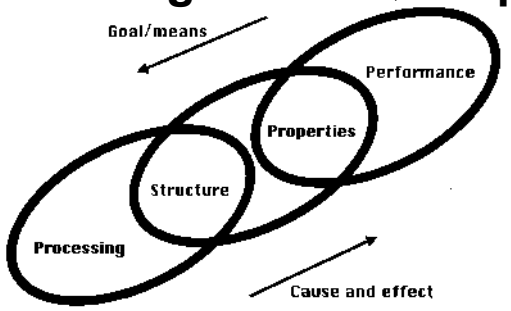
Unfolding Materials Science and Engineering

Scientific Domain Knowledge



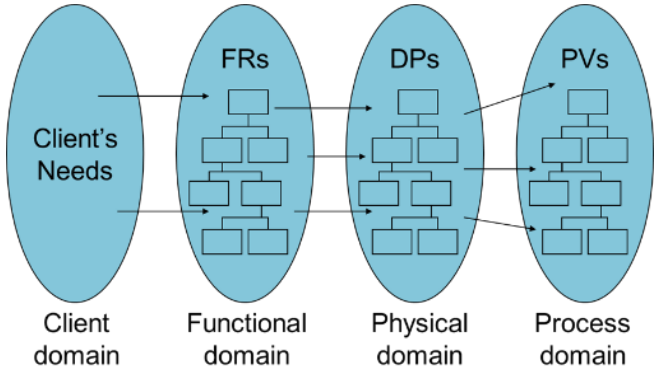
- Undirected hypergraph
- Connections correspond to relationships in literature

Predictive Design Relationships

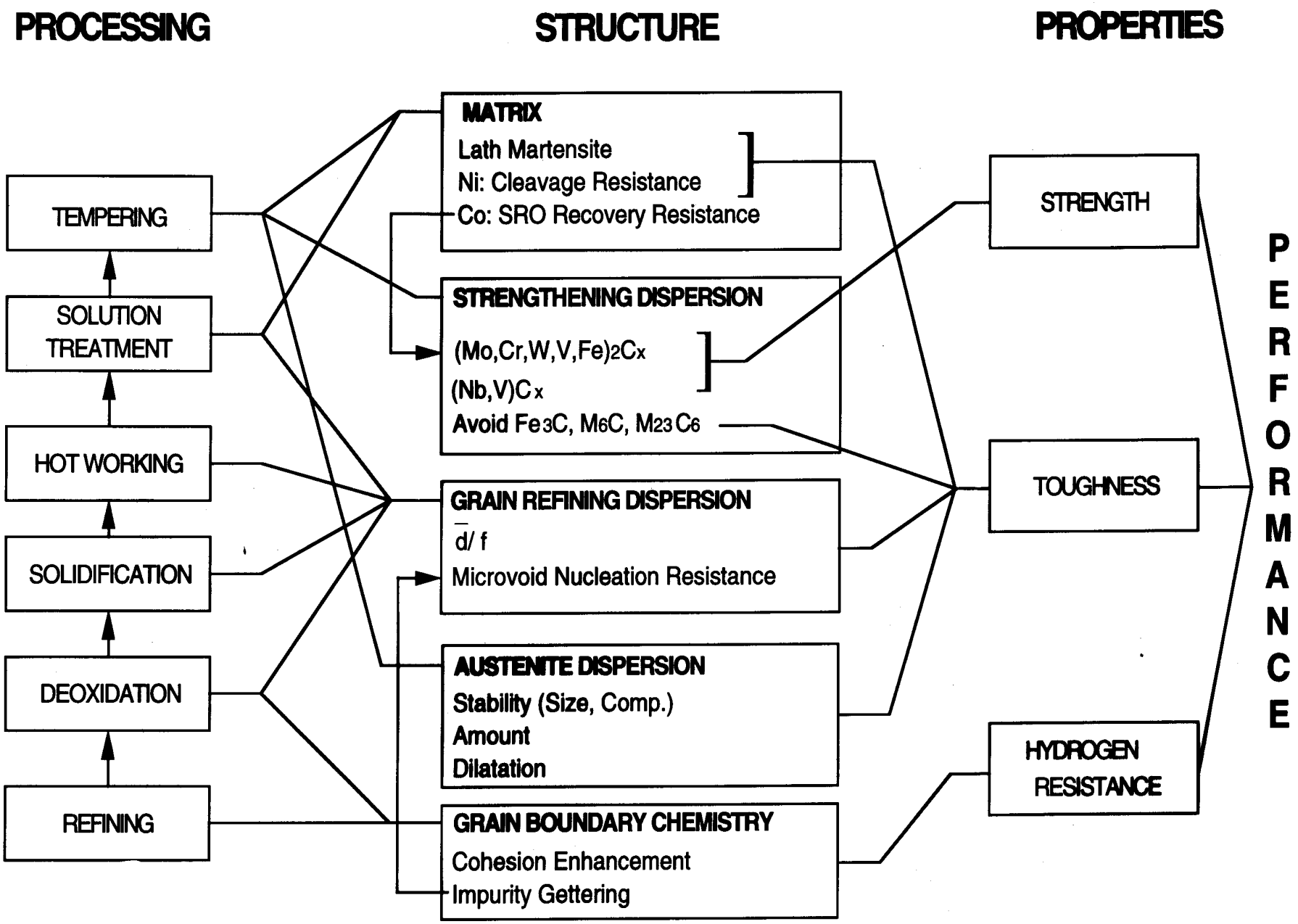


- Undirected graph
- Connections correspond to non-linear functional relationships
  - Can be extrapolated to new materials

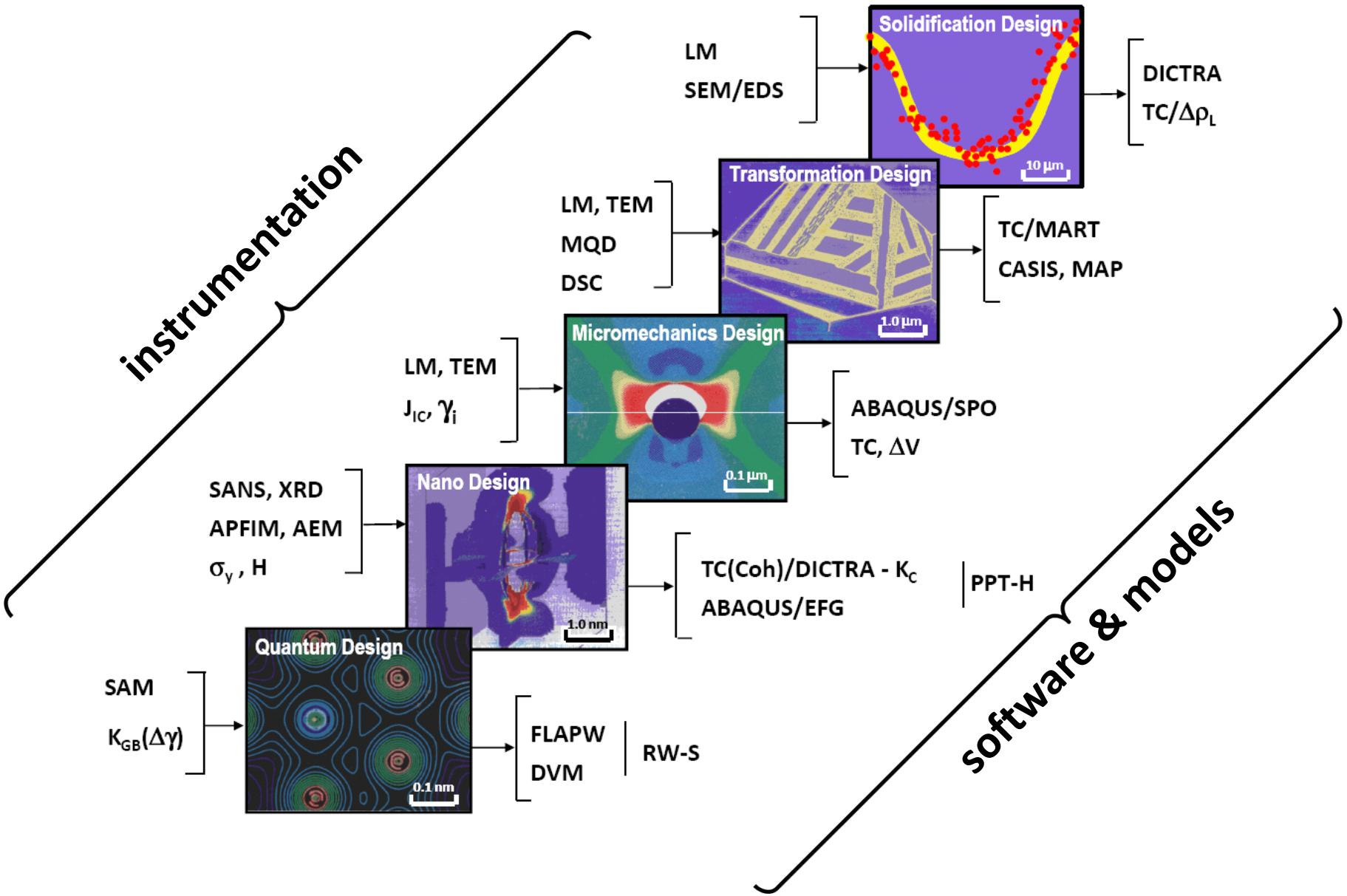
Inverse Process



Nam P. Suh, *"Complexity: theory and applications,"* Oxford university press, 2005.

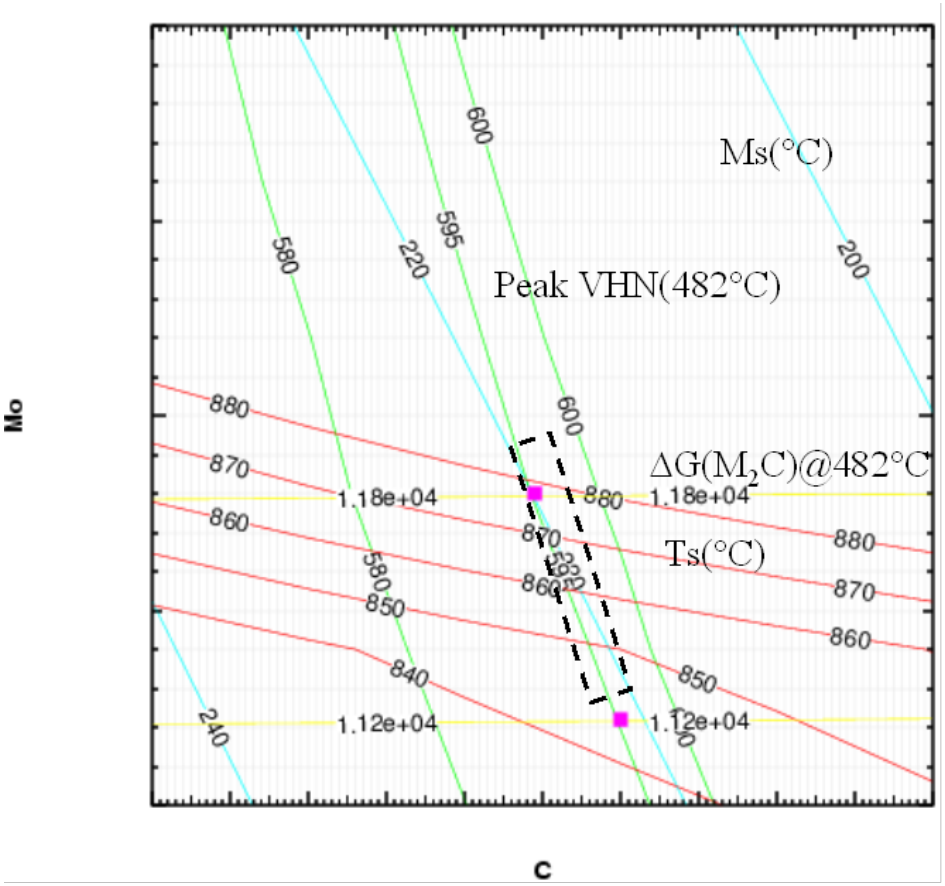

PROCESSING
STRUCTURE
PROPERTIES
TEMPERING
SOLUTION TREATMENT
HOT WORKING
SOLIDIFICATION
DEOXIDATION
REFINING
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
STRENGTHENING DISPERSION
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
GRAIN REFINING DISPERSION
d̄/ f
Microvoid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

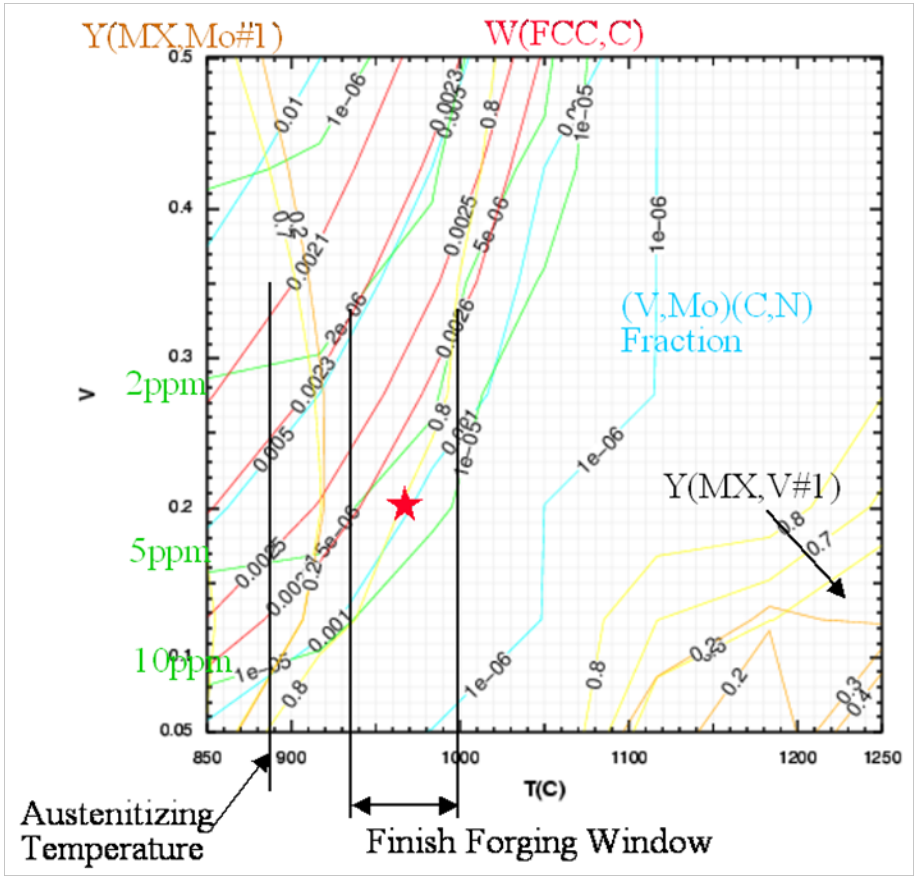


Example: Design Integration with CMD

Matrix + Strengthening Dispersion Design



Grain Pinning Dispersion Design

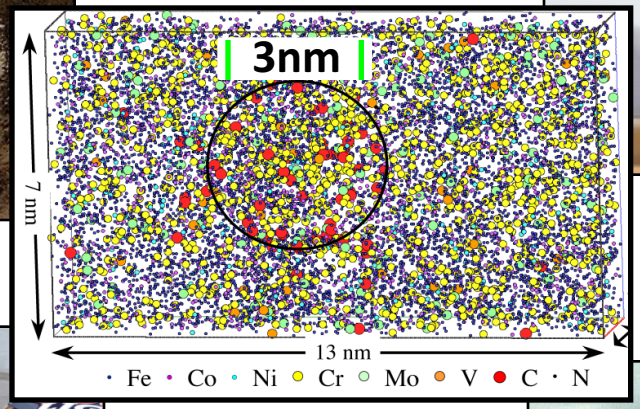


CyberSteels to Market

QuesTek® INNOVATIONS LLC

Ferrium C61 **AMS6517**

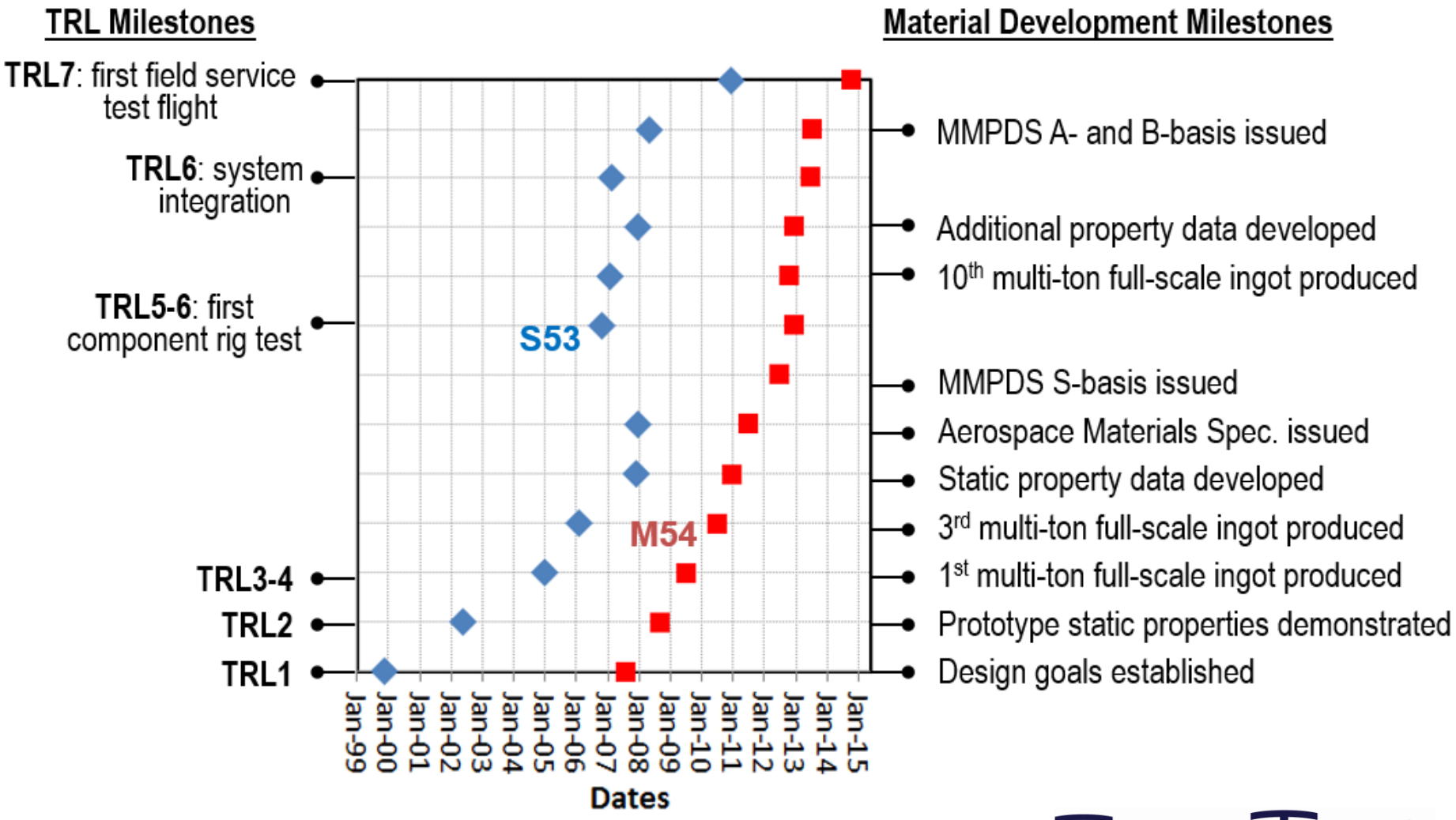
Ferrium S53 Stainless **AMS5922**



Ferrium C64 **AMS6509**

Ferrium M54 **AMS6516**

Computational Materials Qualification Acceleration



QUESTEK® INNOVATIONS LLC

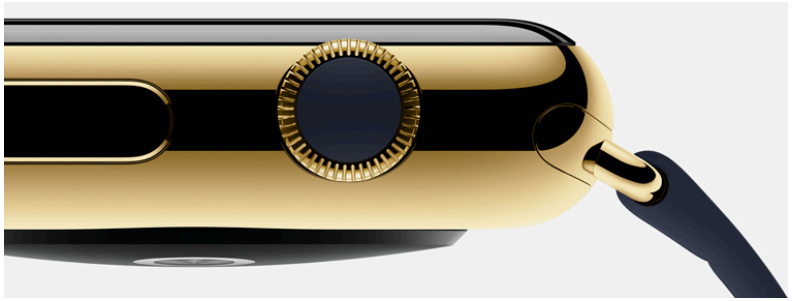
Apple watch

-Announced September 2014

Baseline: 316L Stainless Steel

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

High Strength 18K Gold



-2X harder

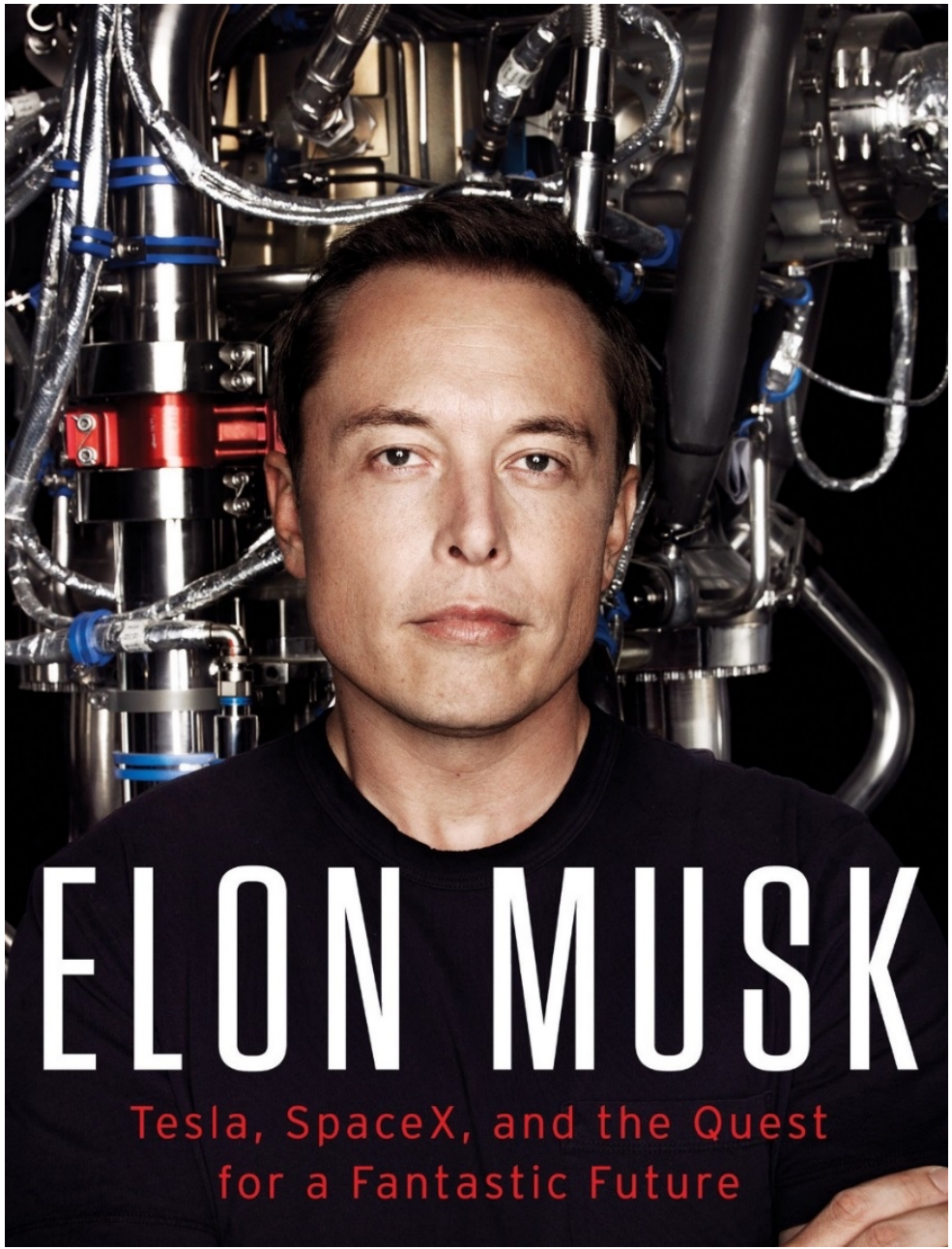
Milanese Loop Alloy

-Custom Magnetic Stainless Steel

Anodizable 7000 Aluminum

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

MGI: From Ferrium Ridge to Silicon Valley



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

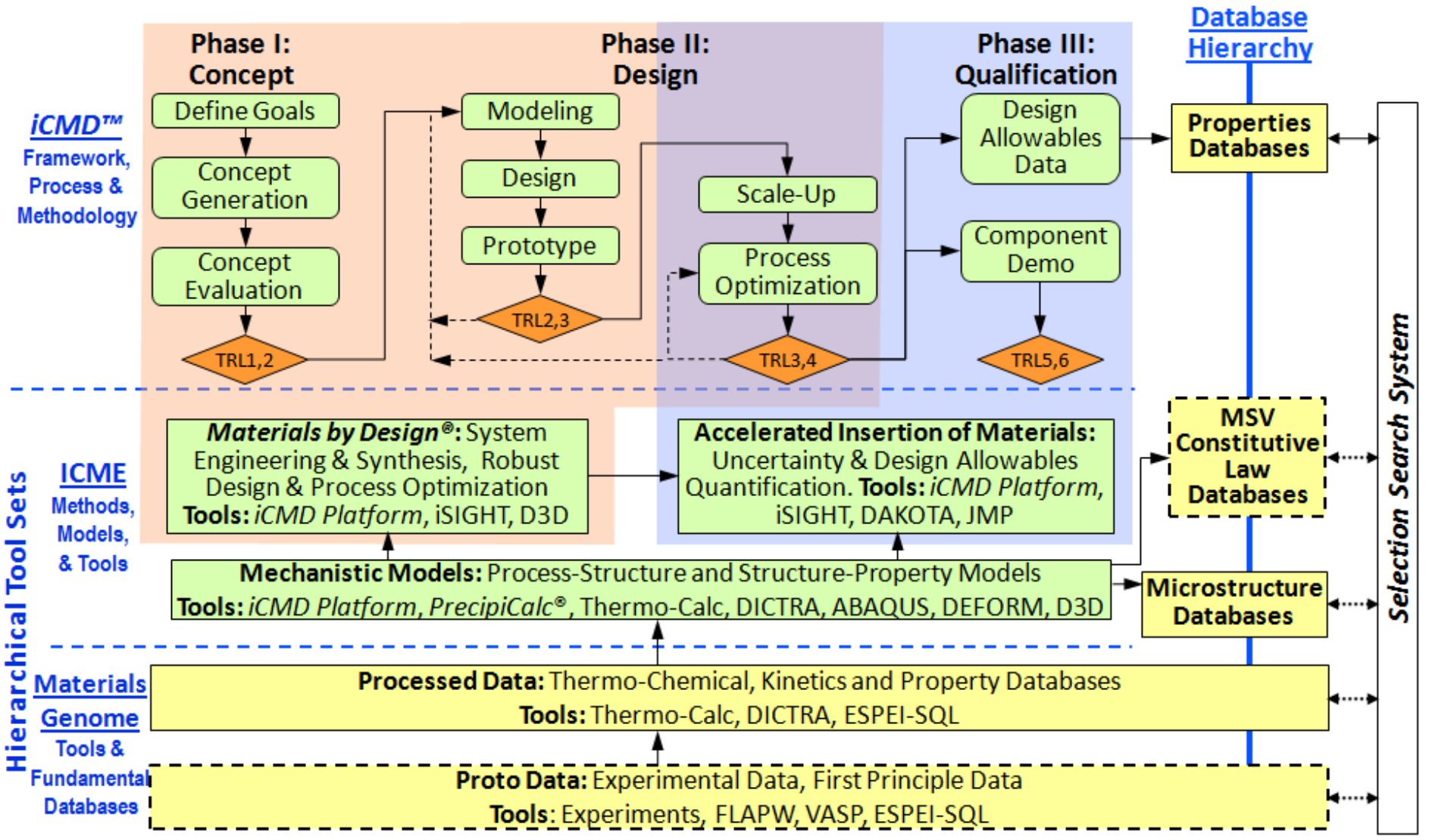
FAYETTEVILLE STATE UNIVERSITY

ASM INTERNATIONAL The Materials Information Society

NIST

CHiMaD

Center for Hierarchical Materials Design



AEC Computational Materials Subcommittee

ASM Materials Genome Toolkit

in collaboration with ThermoCalc Software AB

Software:

Thermo-Calc
DICTRA
TC-PRISMA
TQ-Interface
TC Toolbox for MATLAB
TC-API

Databases:

TCFE + MOBFE (for steels)
TCAL + MOBAL (for Al-alloys)
TCNI + MOBNI (for Ni-alloys)
TCMG (for Mg-alloys)

Pilot Program: Michigan Technological University
Goal: 3yr licenses to 14 undergraduate materials programs

CHiMaD