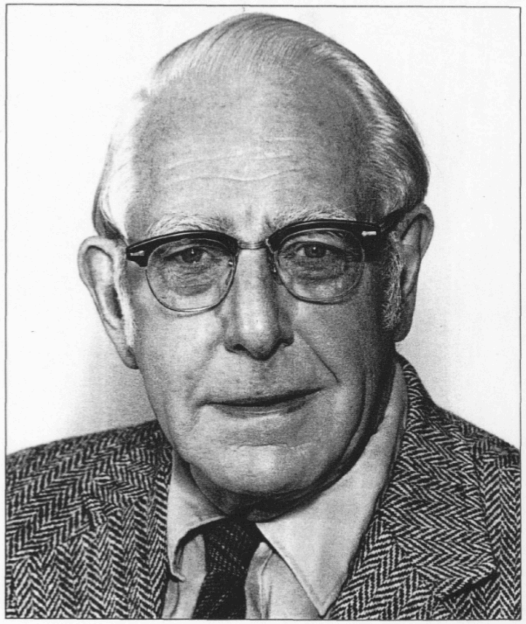
Use Cases:
Inorganic Systems

G. B. Olson

CHiMaD

STRUCTURE- C.S. Smith



Interactive Hierarchy

-Space-Filling Aggregates: materials science, biology, geology

-Perfection/Imperfecton
-Entity/Identity
} duality of description

-"Mesoscopic" Regime

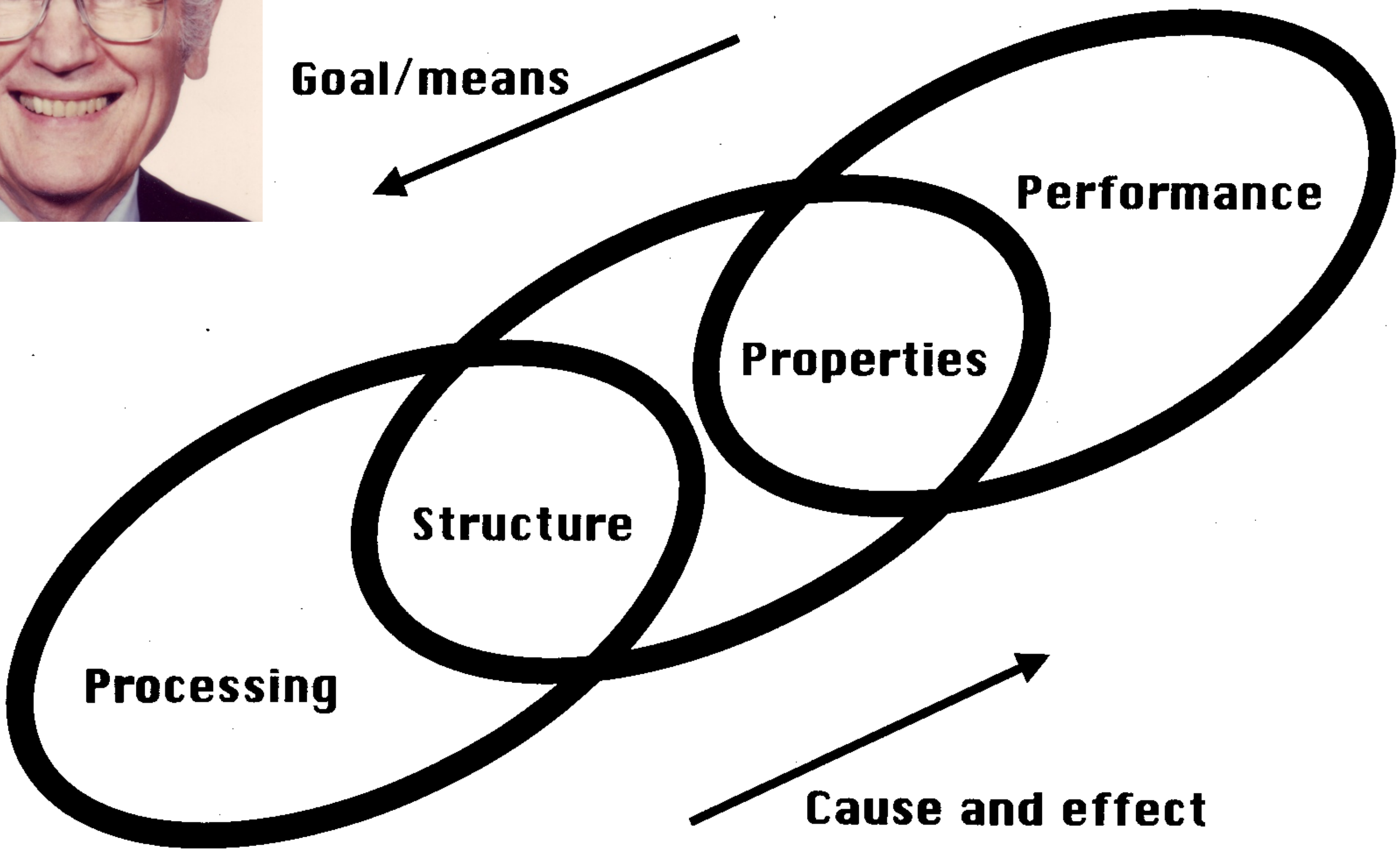
Real Complexity vs. Idealized Simplicity

-Cartesian Corpuscular Philosophy
-Atom/Continuum

Dynamics

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

Cohen's Reciprocity



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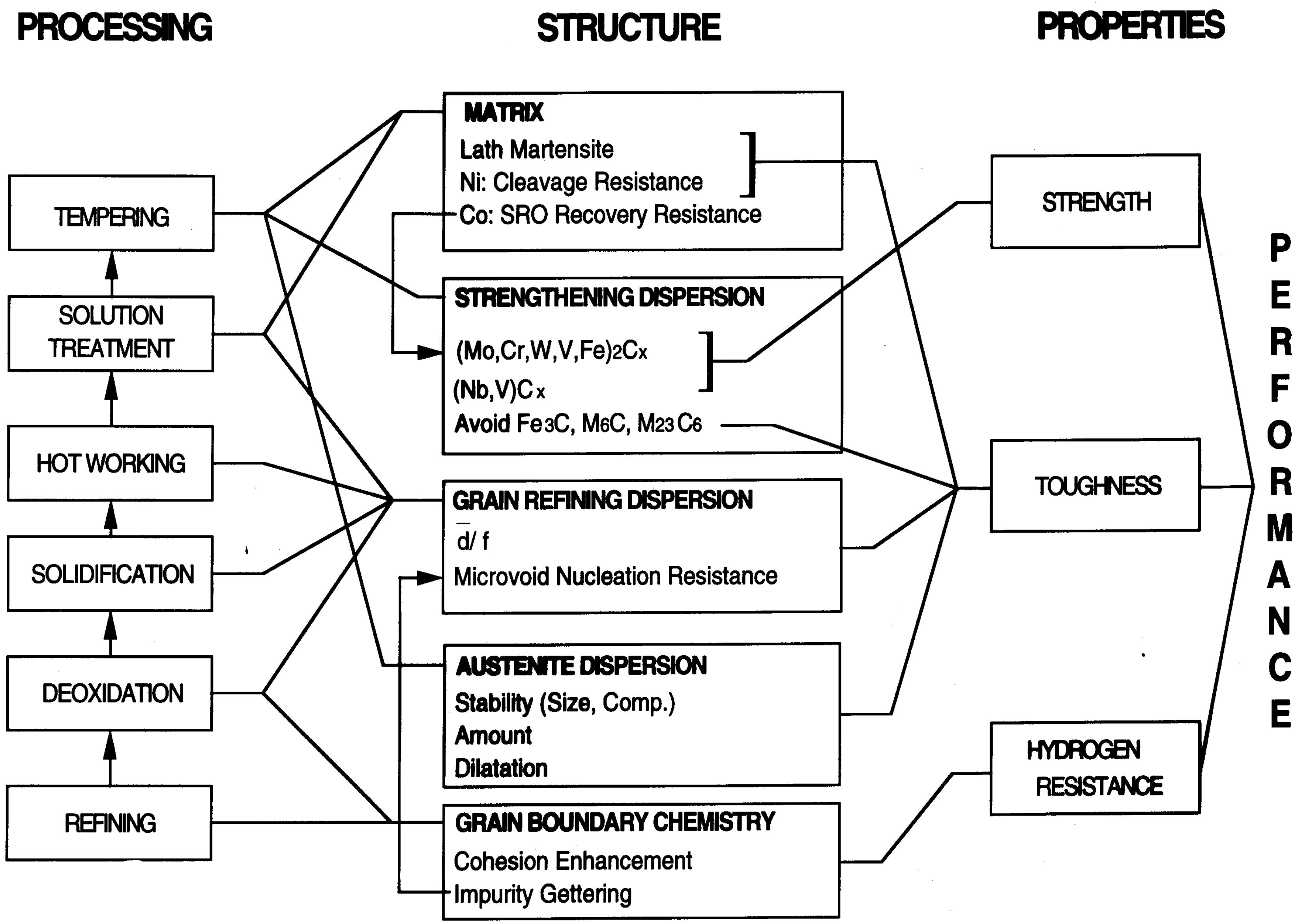
PROCESSING
STRUCTURE
PROPERTIES
TEMPERING
SOLUTION TREATMENT
HOT WORKING
SOLIDIFICATION
DEOXIDATION
REFINING
MATRIX
Lath Martensite
Ni: Cleavage Resistance
Co: SRO Recovery Resistance
STRENGTHENING DISPERSION
(Mo,Cr,W,V,Fe)2Cx
(Nb,V)Cx
Avoid Fe3C, M6C, M23C6
GRAIN REFINING DISPERSION
d/ f
Microvoid Nucleation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

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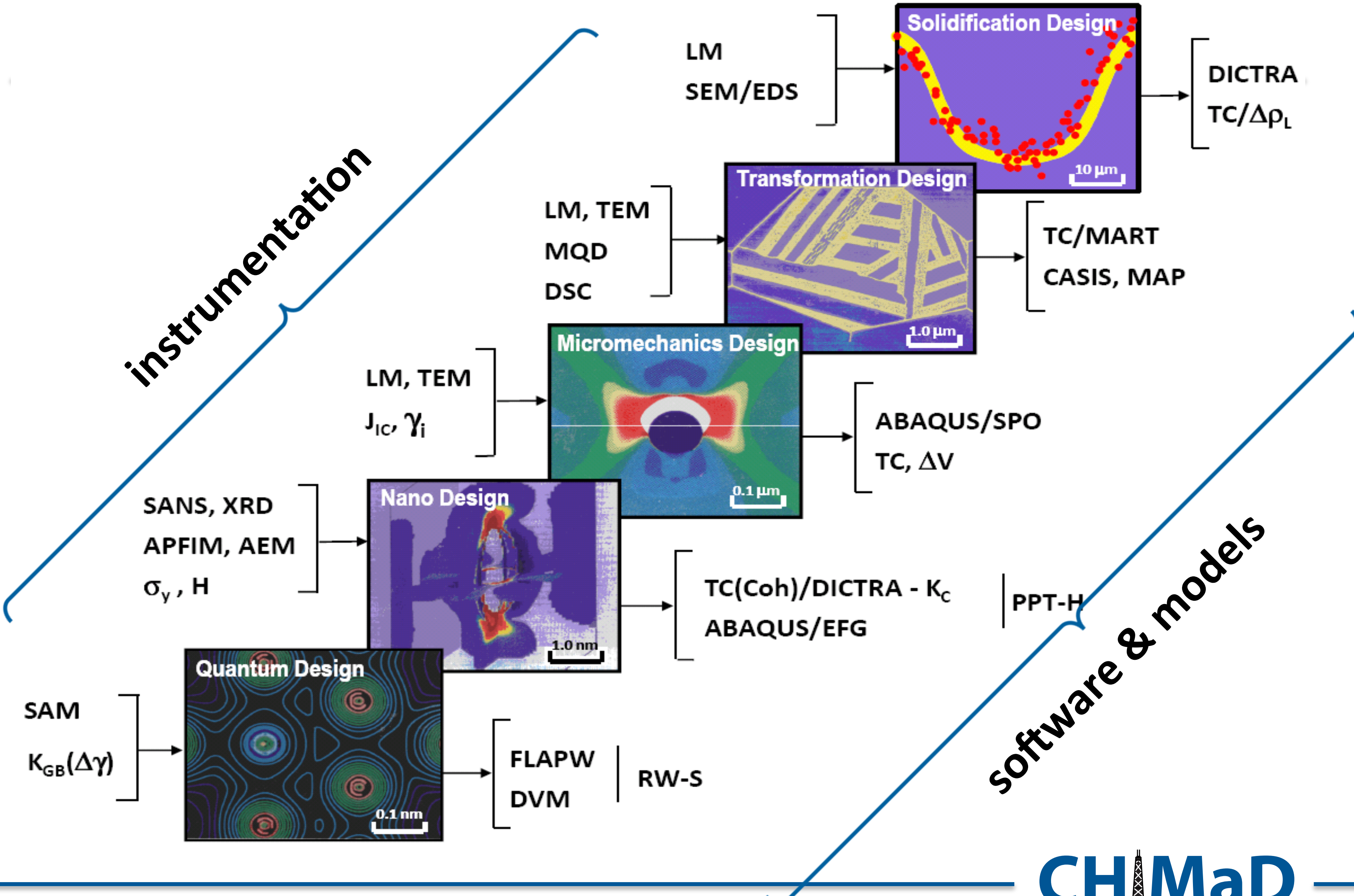
Hierarchy of Design Models



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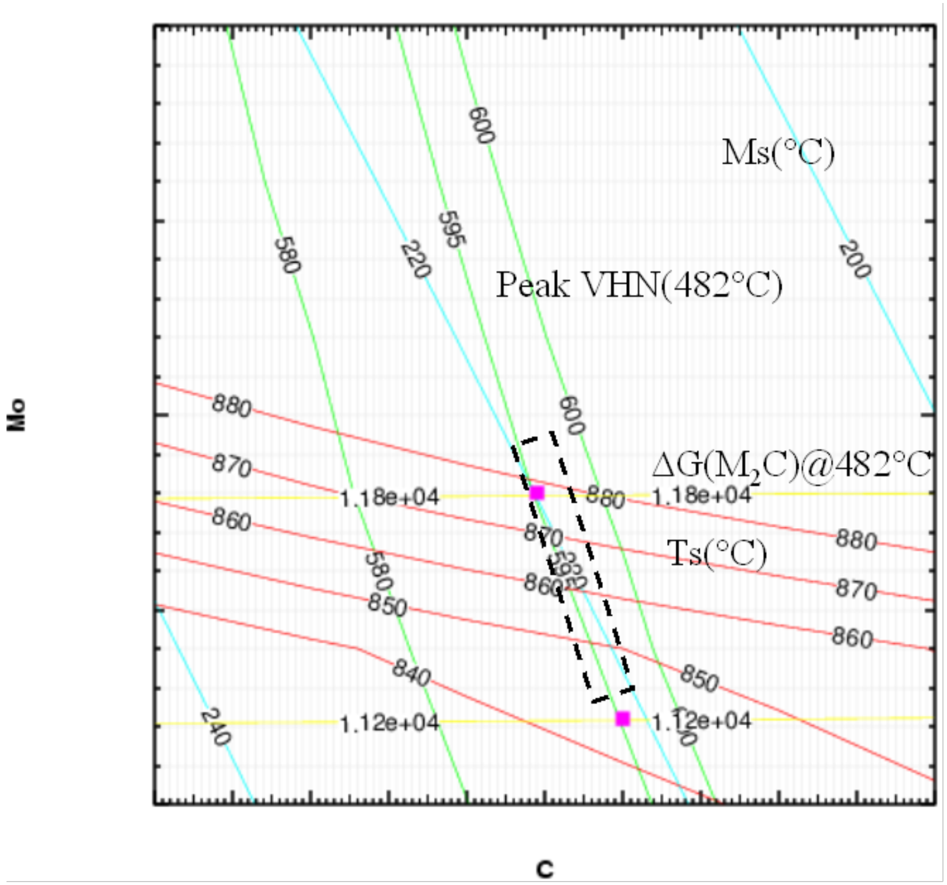
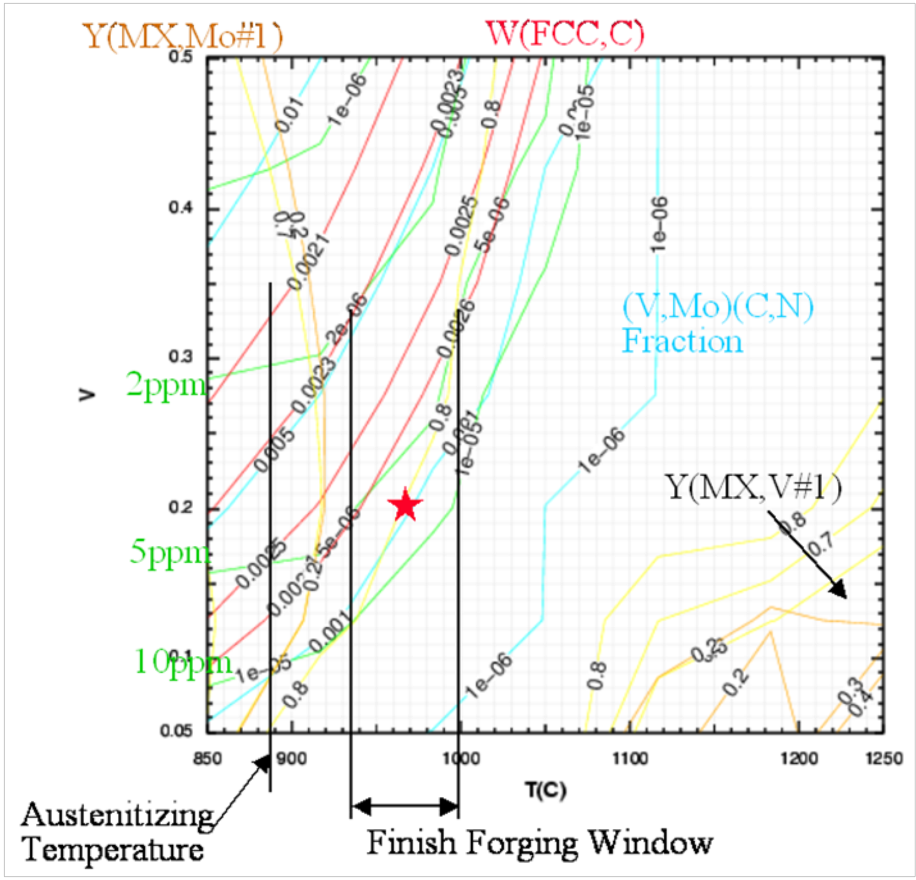
Example: Parametric Design with CMD

Matrix + Strengthening Dispersion Design

Grain Pinning Dispersion Design





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Hard Material Use-Case Groups

- Cobalt alloys
- Nanodispersion-strengthened shape memory alloys
- Si-based insitu composites
- Leveraging: Steel Research Group projects

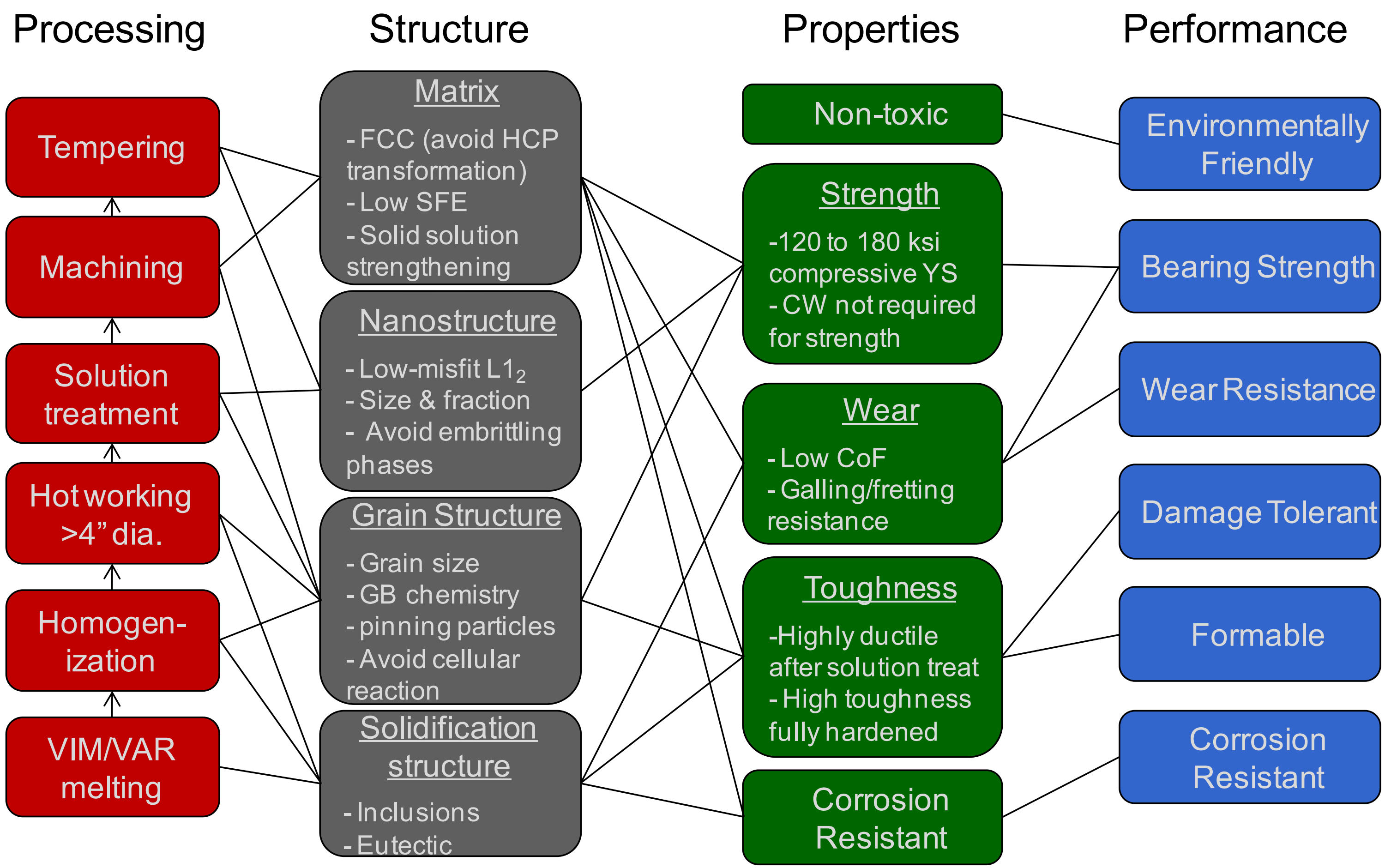
Cobalt Alloy Designs

G. Olson (NU), D. Dunand (NU), D. Seidman (NU), P. Voorhees (NU), M. Stan (NAISE, ANL) C. Wolverton (NU)

- Motivation:
  - Need turbine blade alloys that exceed the use temperatures of Ni-based superalloys
  - Wear resistant ambient temperature applications to replace Be-Cu

- Goals:
  - Near-term: Ambient temperature bushing alloy
  - Long-term: High-temperature aeroturbine superalloy

PH Cobalt System Chart



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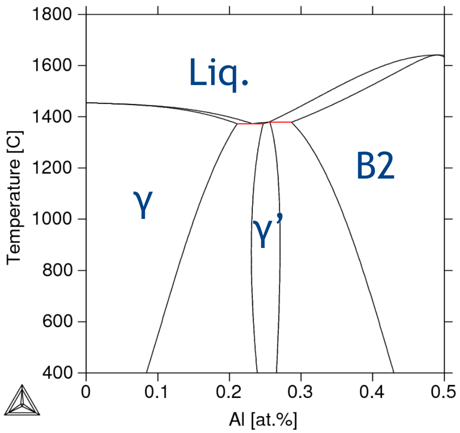
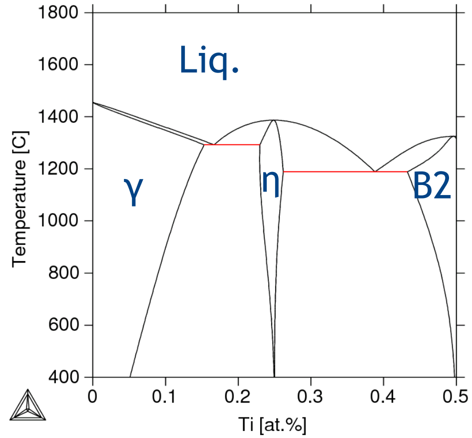
$L1_2$ Stability in Ni vs Co Systems

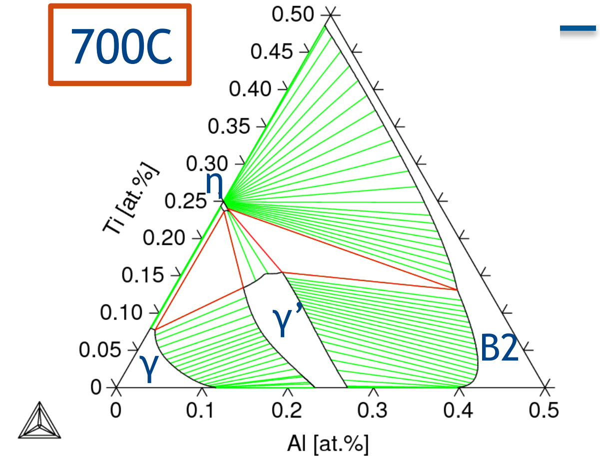
Ni



Ni-Al

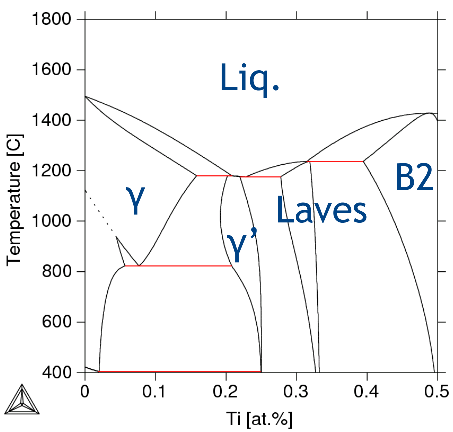


Ni-Ti

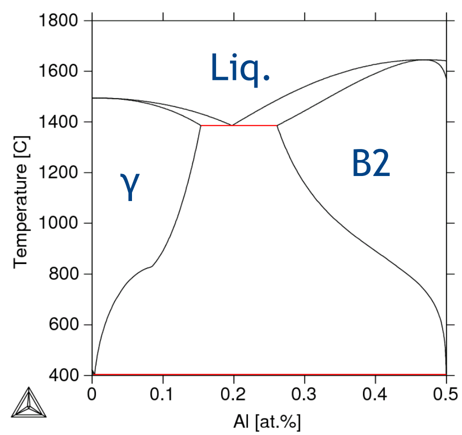


Ni-Al-Ti

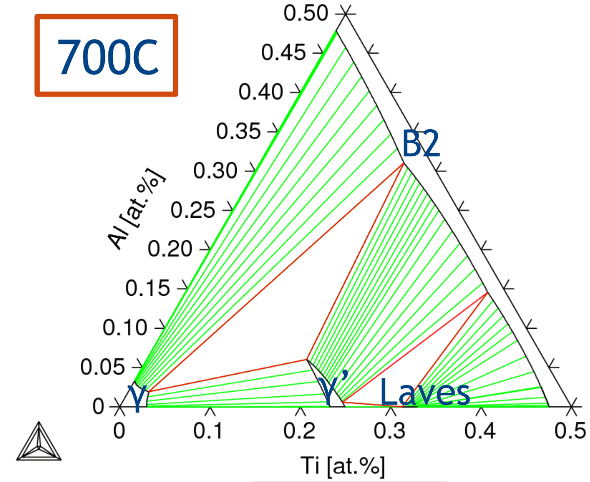
Co



Co-Ti

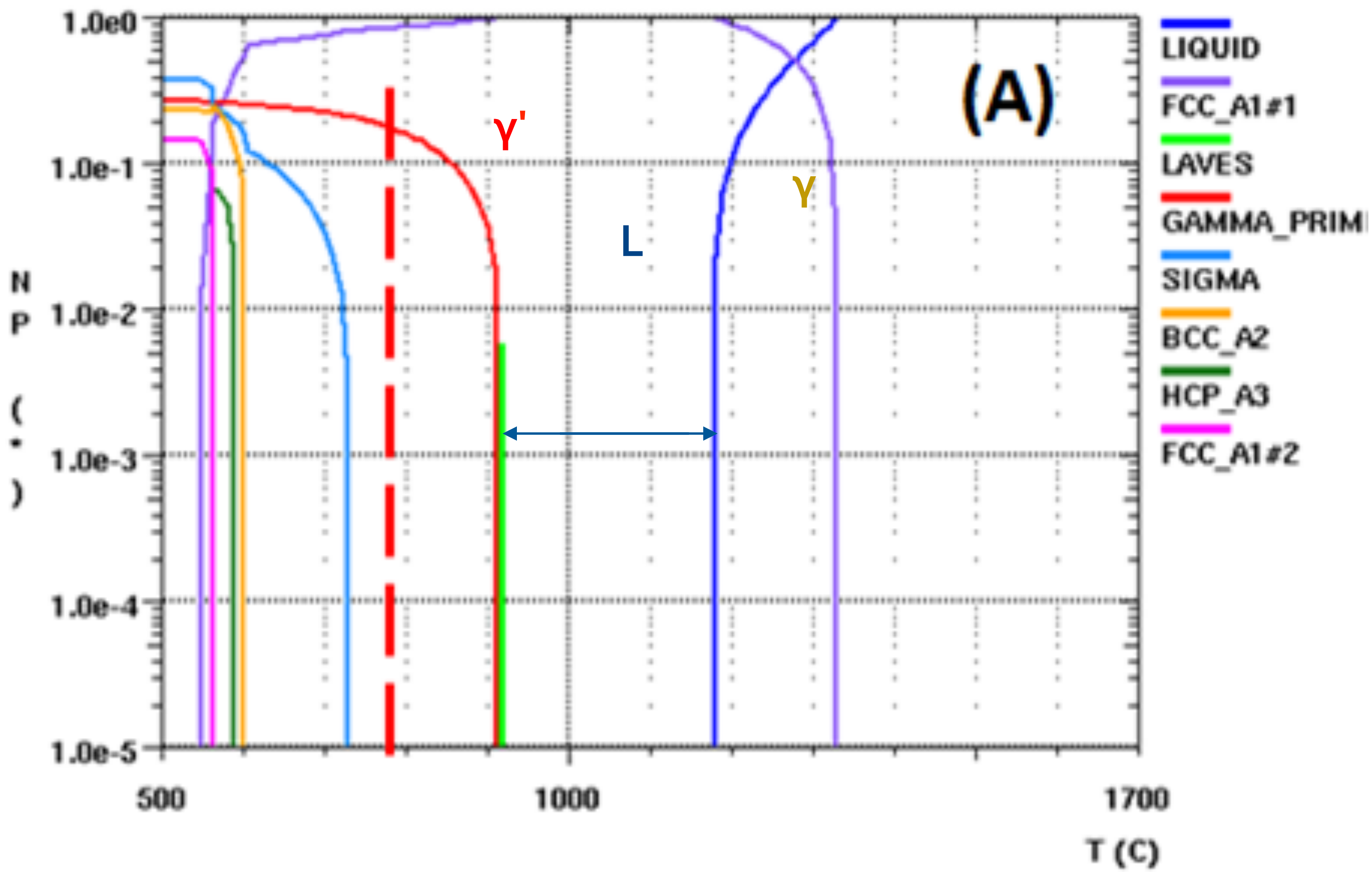


Co-Al



Co-Ti-Al

CALPHAD Step Diagram



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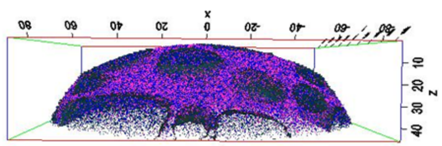
Validation of design with LEAP characterization

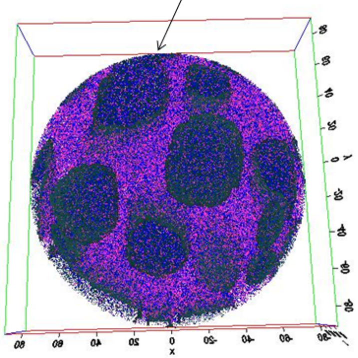
LEAP validation of alloy nanostructure after tempering at ~780˚C:
FCC (Co-rich) matrix and γ' [$L1_2$ crystal structure, $(Co,Ni)_3(Ti,V)$-type] strengthening nanoprecipitates

- 21.2M ions, 46 x 181 x 179 nm^3

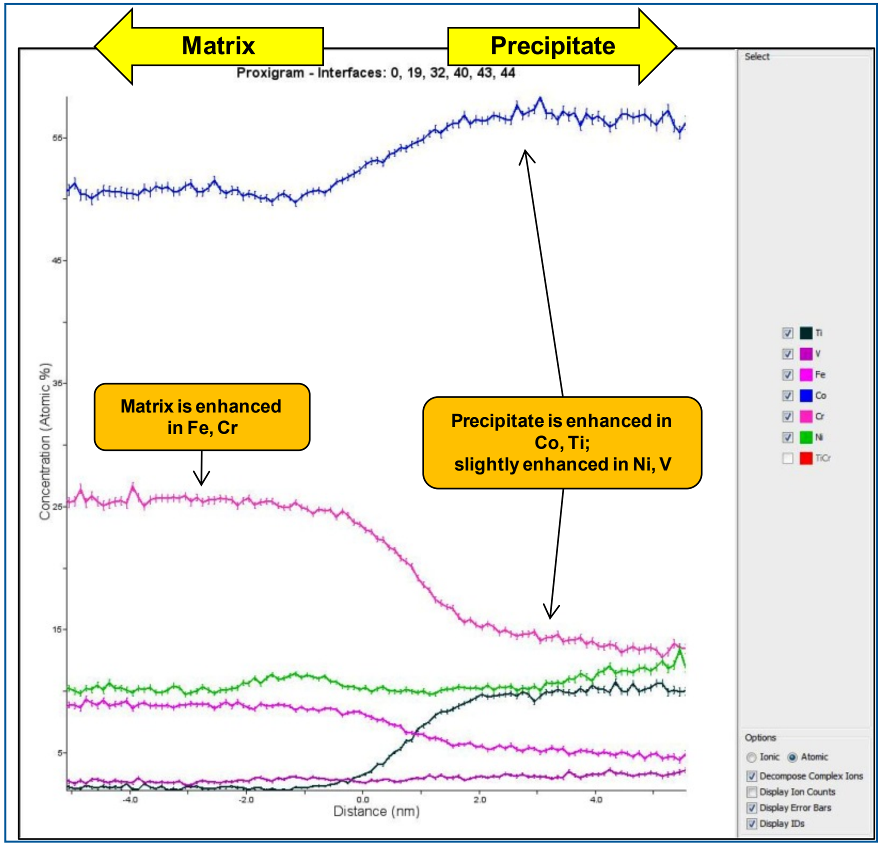


Side view

~40-50 nm diameter $L1_2$ precipitates



Top view



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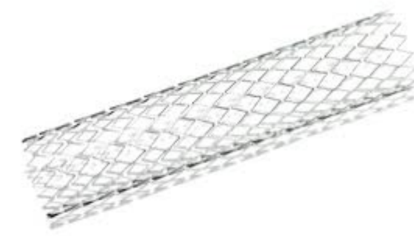
Approach

- Years 1 and 2:
  - Accelerated expansion of Co system multicomponent solution thermodynamics, molar volume, and diffusivity databases (high throughput theory and experiment) to incorporate Nb, Mo, Ta, Re and B for FCC, L12 and L phases.
  - LEAP microanalytical calibration and validation.
- Years 3 and 4
  - Prototype alloy validation and preliminary process optimization
  - PrecipiCalc calibration and application to detailed process optimization
  - Solidification and homogenization modeling for scale-up
  - Continuum modeling of creep deformation dynamics
  - Neutron and X-ray diffraction evaluation of load partitioning

Nanodispersion-Strengthened Shape Memory Alloys

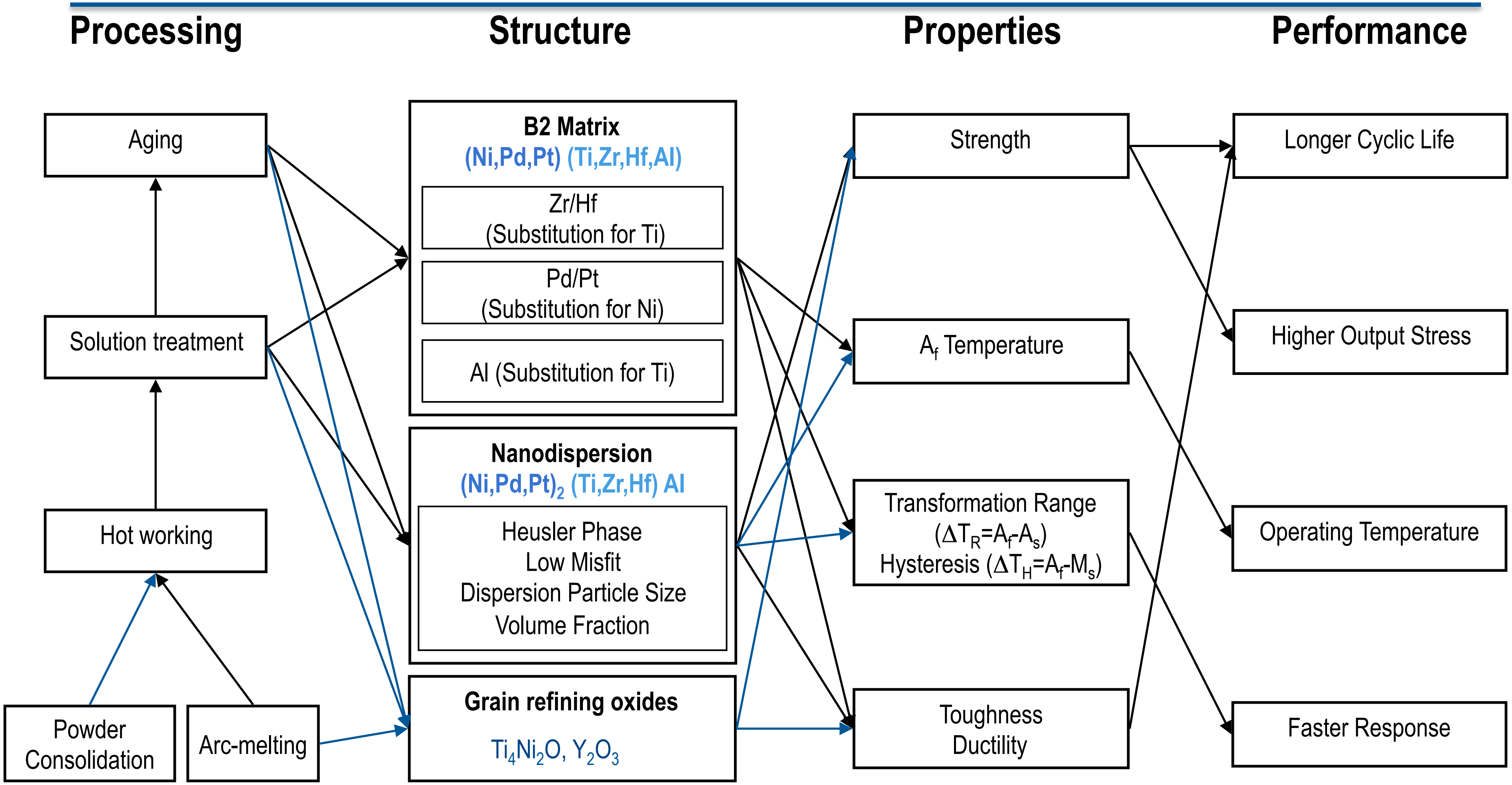
G. Olson (NU), D. Dunand (NU),W-K. Liu (NU) D. Seidman (NU),
A. Umantsev (FS), C. Wolverton (NU)

- Motivation:
  - Widely used in medical, aerospace and automotive sectors
  - Current alloys are susceptible to instability after many cycles



- Goals:
  - Near-term: Pd-stabilized alloys for medical devices
  - Long-term: High-temperature aeroturbine & automotive actuators

SMA System Chart



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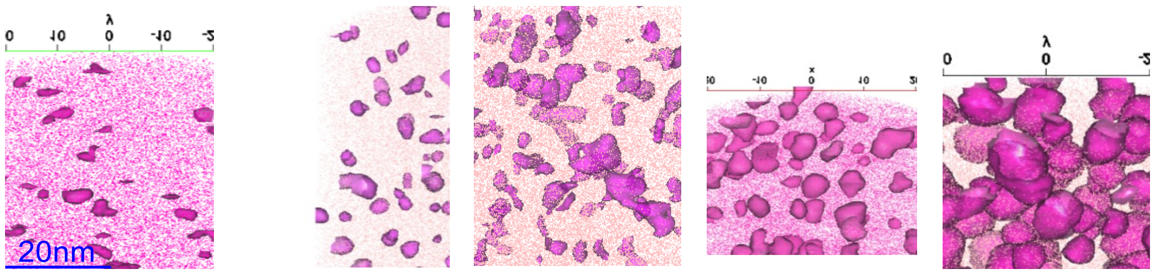
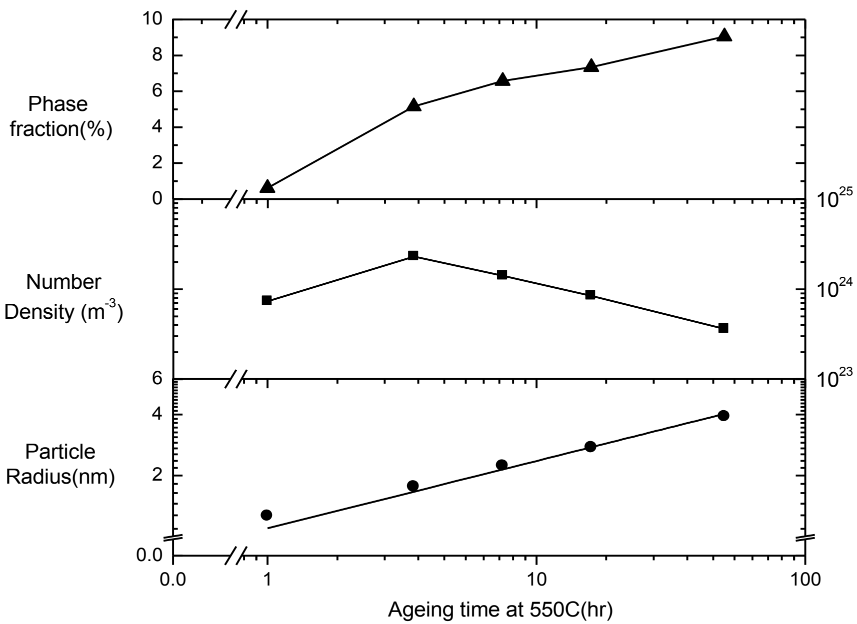
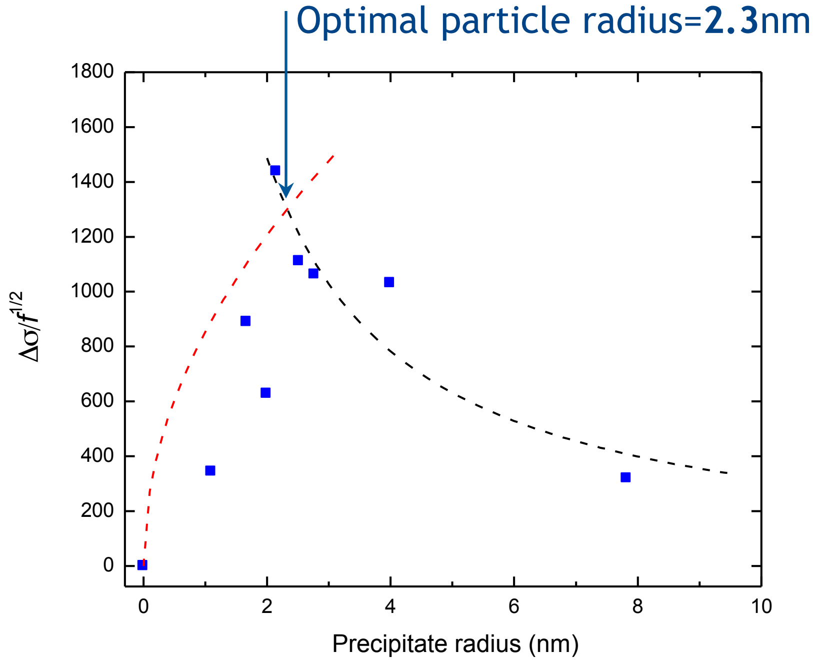
Precipitation strengthening in $(Pd,Ni)_{50}(Ti,Al)_{50}$ alloys

Ageing at 550°C

1hr 3.5hr 7.5hr 16hr 50hr



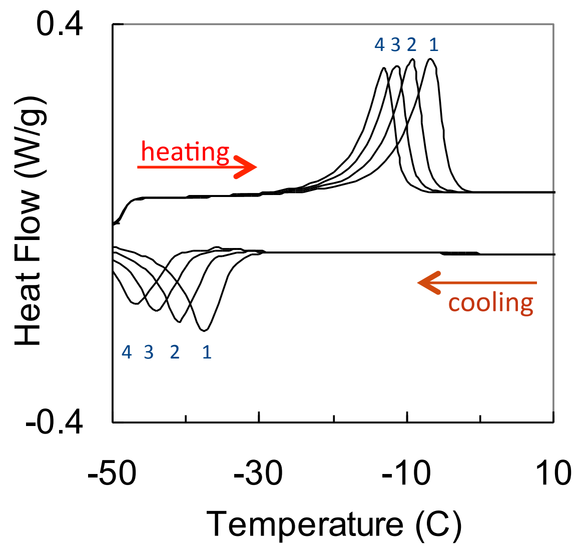




SMA Cyclic Stability

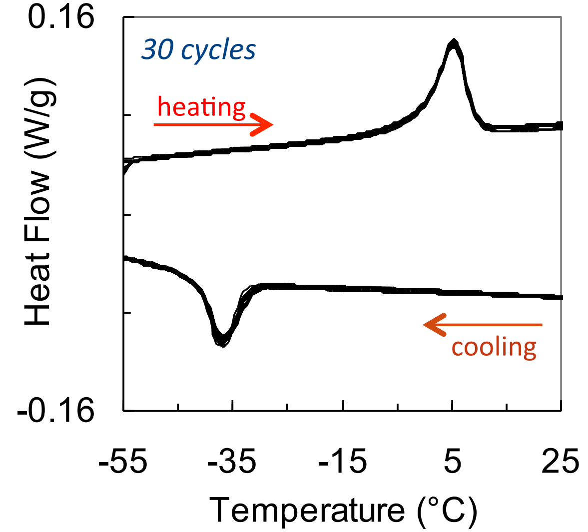
Thermal cyclic stability

$Ti_{49.3}Ni_{50.8}$

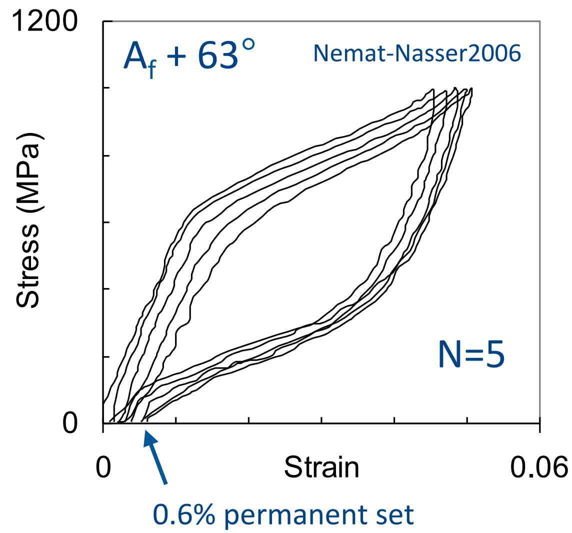


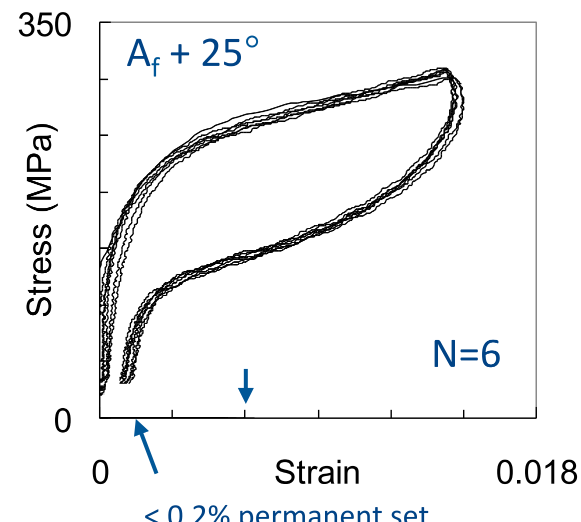
$Ni_{20}Pd_{30}Ti_{46}Al_4$

Aged 600°C, 5h



Mechanical cyclic stability (compression)





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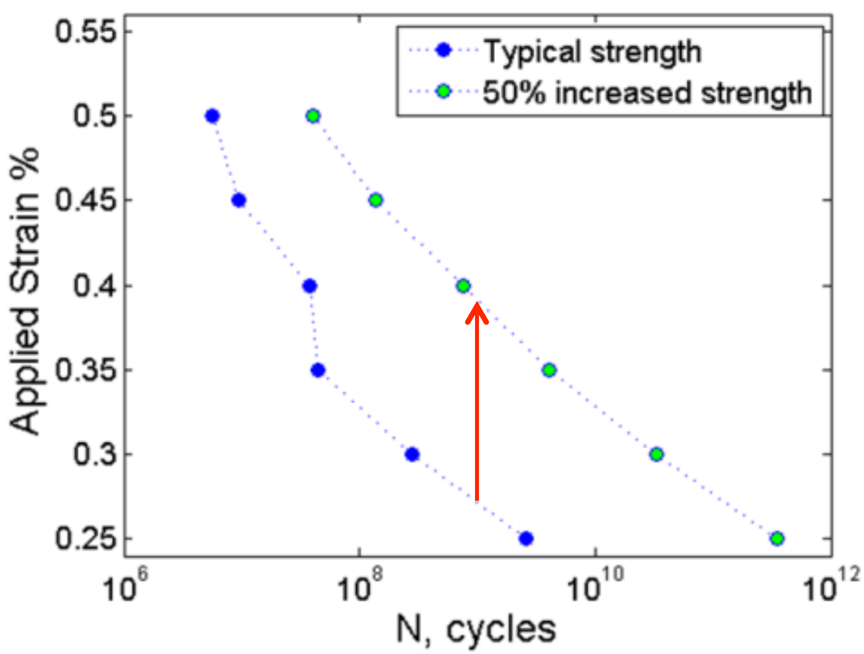
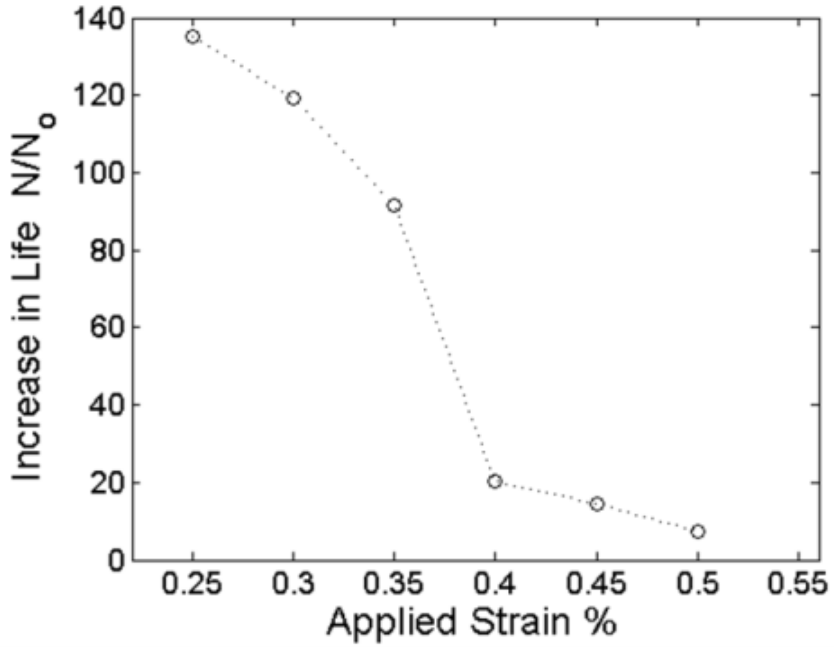
TiNi Fatigue Life Prediction:
Effect of Increased B2 Strength

Increased life (N) of strengthened alloy compared typical life (N_o)





- **50% increase in matrix strength** results in increase in fatigue limit (at 10^9 cycles) from **0.27%** to **0.39%**
- Benefit of B2 strengthening increases as applied strain decrease

Approach

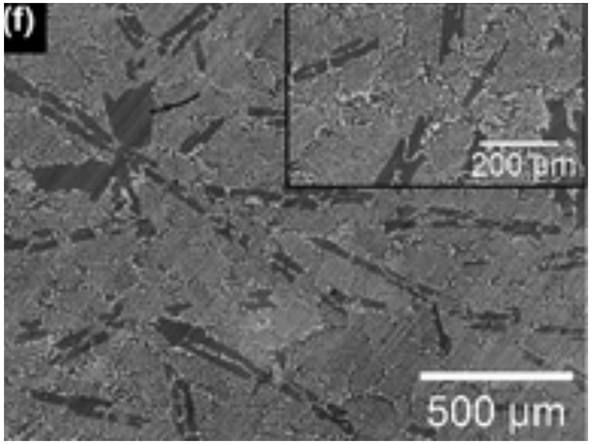
- Years 1 and 2:
  - Accelerated expansion of solution thermodynamics, molar volume, and diffusivity database (high throughput theory and experiment) of Ti-Zr-Hf-Ni-Pd-Pt-Fe-Co-Ni-Al-O-C system for B2, L21, M(O,C), M6O, and martensitic phases
  - LEAP microanalysis calibration and validation
  - D3D characterization of fatigue nucleants and ABC continuum modeling of fatigue nucleation

- Years 3 and 4
  - Prototype evaluation and preliminary process optimization
  - PrecipiCalc calibration and application to process optimization
  - ABC continuum modeling of oxide and carbide evolution during deformation processing
  - Solidification and homogenization modeling for process scale-up

In-Situ Si Composite Materials

P. Voorhees (NU), J. De Pablo (UC), W. Chen (NU),
S. Davis (NU) , C. Wolverton (NU)

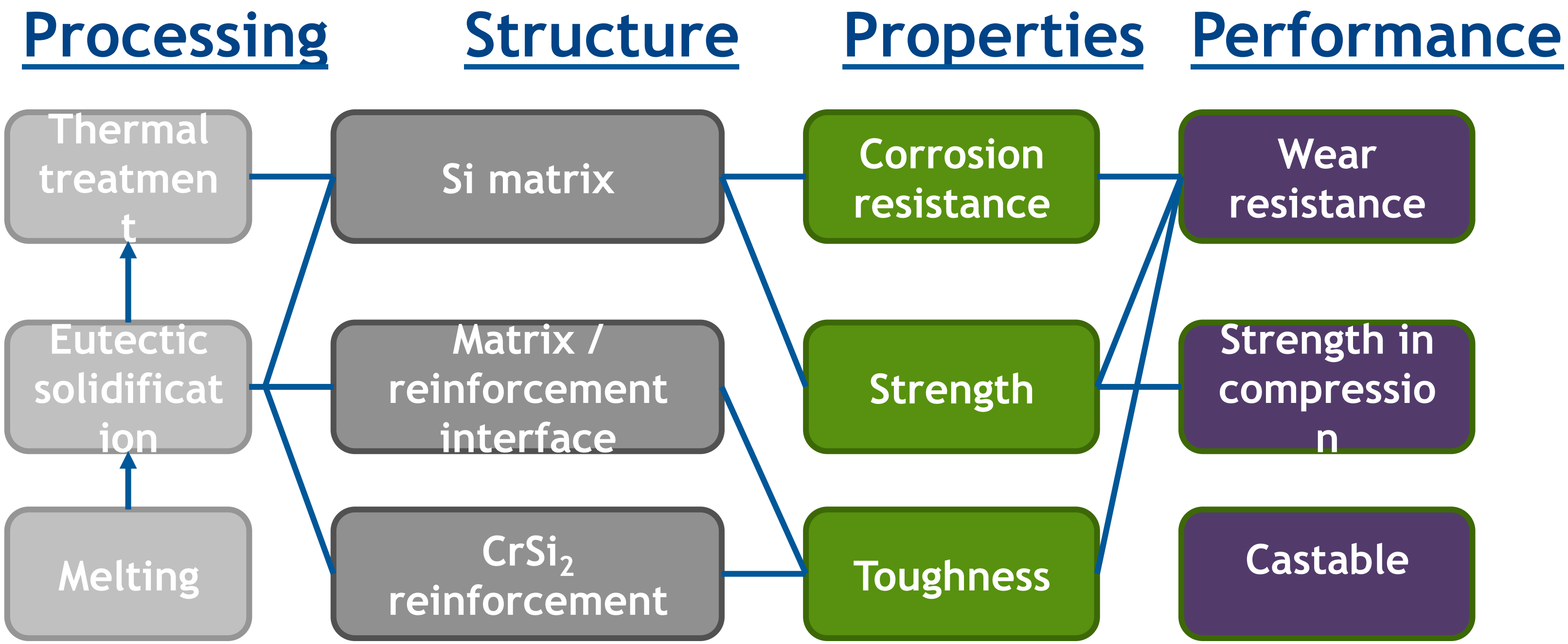
- Motivation:
  - Corrosion resistant, tough alloys
  - Avoid the complications of classical ceramic processing, such as sintering
  - Employ insitu Si-composites
- Goals:
  - Near-term: A multicomponent eutectic growth model
  - Long-term: A tough, castable Si alloy



Si-$CrSi_2$ composite
(Fischer and Schuh, J. Am Ceram. Soc, 2012)

Design Approach

- Primary mechanism of toughening is the delamination of interphase interfaces
- Composites are produced via eutectic solidification
- Industrial partner: Dow Corning



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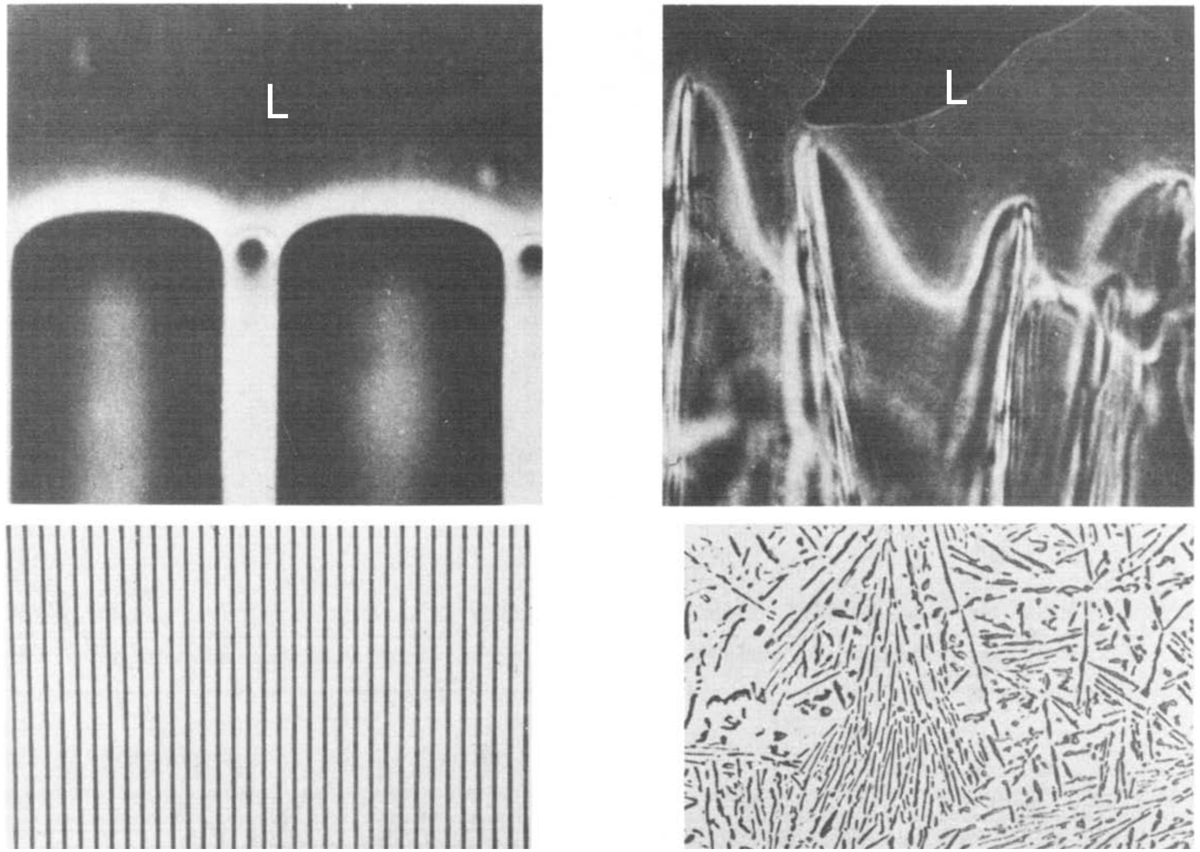
Growth of Si Composites

Due to the anisotropy of the solid-liquid interfacial energy, Si alloys can grow as irregular eutectics



Al-Si

Isotropic

Anisotropic

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Approach

- Years 1 and 2:
  - Use multicomponent thermodynamics to inform eutectic growth models
  - Generalize eutectic growth models to multicomponent systems, use existing corrections for anisotropic interfacial energy
  - Predict solidification paths, and thus volume fractions of phases, and length scales of the solidified morphologies
- Years 3 and 4
  - Phase field models for systems with highly anisotropic solid-liquid interfacial energy
  - Develop descriptors of the microstructure
  - Using these descriptors, and models of the toughening process, design optimal microstructures
  - Using models for the multicomponent eutectic solidification process develop optimal microstructures
  - Characterization using X-ray tomography

2014 SRG Design Projects

- **ONR Cyberalloys** (Olson, Freeman)
  - CMD of Fe & Ti alloys for blast and fragment protection
- **DOE/GM Lightweighting Initiative** (Olson, Wolverton, Voorhees)
  - CMD of cast aluminum for cylinder heads
- **DOE/CAT Lightweighting Initiative** (Olson, Liu)
  - CMD of cast steels for crankshafts
- **ArcelorMittal AHSS** (Olson)
  - CMD of high-strength automotive Q&P TRIP steels
- **NIST/NIU MSAM Additive Manufacturing** (Olson, Liu, Cao)
  - CMD of Fe & Ti alloys for additive manufacturing

DARPA/Honeywell Open Manufacturing (QuesTek)
  - ICME for SLM additive manufacturing of Ni 718+