NIST Center of Excellence:
Advanced Materials

CHiMaD

CENTER FOR HIERARCHICAL MATERIALS DESIGN

Shared Vision

- Realize the full impact of the Materials Genome Initiative to accelerate materials discovery and development
- Demonstrate the power and potential of bringing together data science, computational approaches, and state-of-the-art experiments to design materials
- Build broad research and outreach programs in partnership with government, industry, and academia

Leadership

Peter Voorhees
Northwestern University

Greg Olson
Northwestern University

Juan de Pablo
University of Chicago

Jim Warren
Materials Genome Initiative

Laurie Locascio
Material Measurement Laboratory

Eric Lin
Materials Science and Engineering Division

Approach

- **Leverage** significant strengths and a long history of materials design and collaborative research

- **Identify** thrust areas (use-cases) that:
  - focus on particular materials of industrial and scientific importance
  - involve industrial collaborators
  - transfer the design methodology to industry and other stakeholders

- **Develop**:
  - community standard codes for both hard and soft materials design
  - materials databases that are motivated by topics of the use groups
  - experimental methods for rapid assessment of materials properties

- **Convene** workshops and outreach activities on issues that are central to the implementation of the Materials Genome Initiative

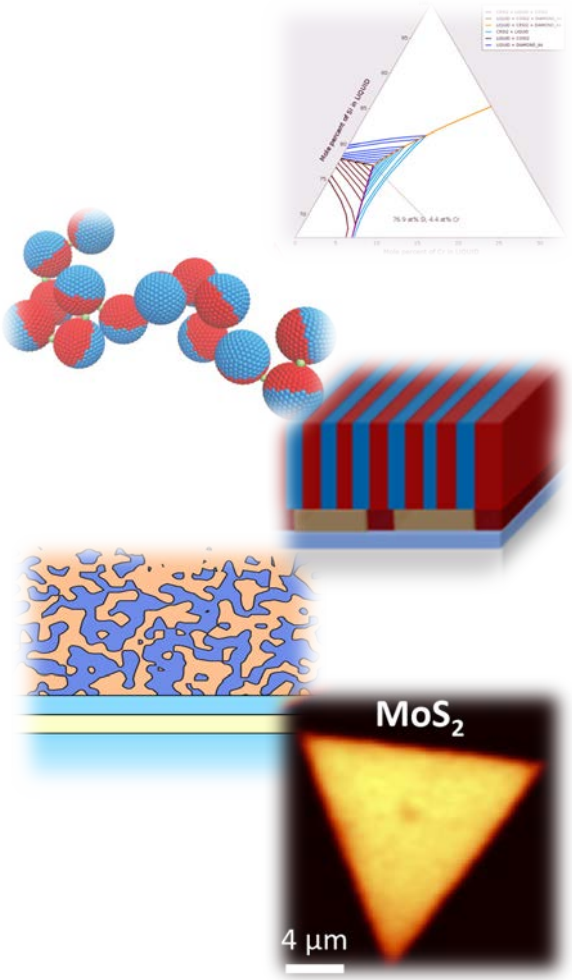
Program Elements

Use-Case Teams:

- Precipitation-Strengthened Alloys
- In-situ Silicon-Composite Materials
- 2D Heterostructures for Electronics
- Polymer Matrix Composites
- Directed Assembly of Block Copolymers
- Polyelectrolyte Self-Assembly
- Organic Polymer Solar Cells
- Data Mining

Cross-cutting Tools:

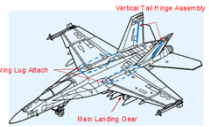
- Software: Standard Phase Field Methods
- Software: Coarse Grained Simulations
- Data: CALPHAD Protodata Databases
- Data: Materials Data Facility
- Expt: Resonant Soft X-ray scattering
- Expt: Rapid Assessment of Phase Relations



PRECIPITATION-STRENGTHENED ALLOYS: Co-based

DESIGN GOALS

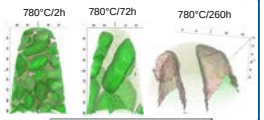
- *Apply accelerated insertion of materials (AIM) approach for accelerated qualification of precipitation-strengthened Co-based bushing/actuator alloy use case*



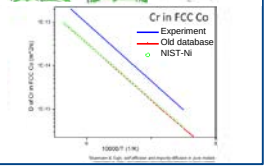
QuesTek Co Alloy:
Designed and developed an environmentally safe drop-in alternative alloy as a substitution for highly loaded bushing applications.

Databases calibrated with experimentation

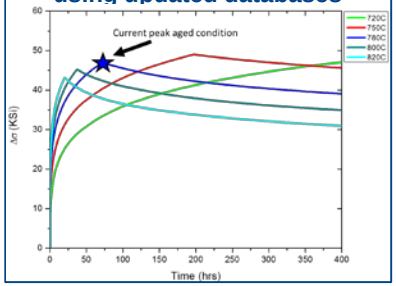
Thermodynamic database refined with Atom Probe Tomography



Kinetic database refined with literature diffusivity data

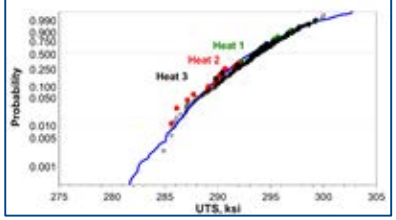


Calibrated strength modeling using updated databases



New material procured (process optimization in process)

Next step: AIM simulations (strength) and targeted experimentation

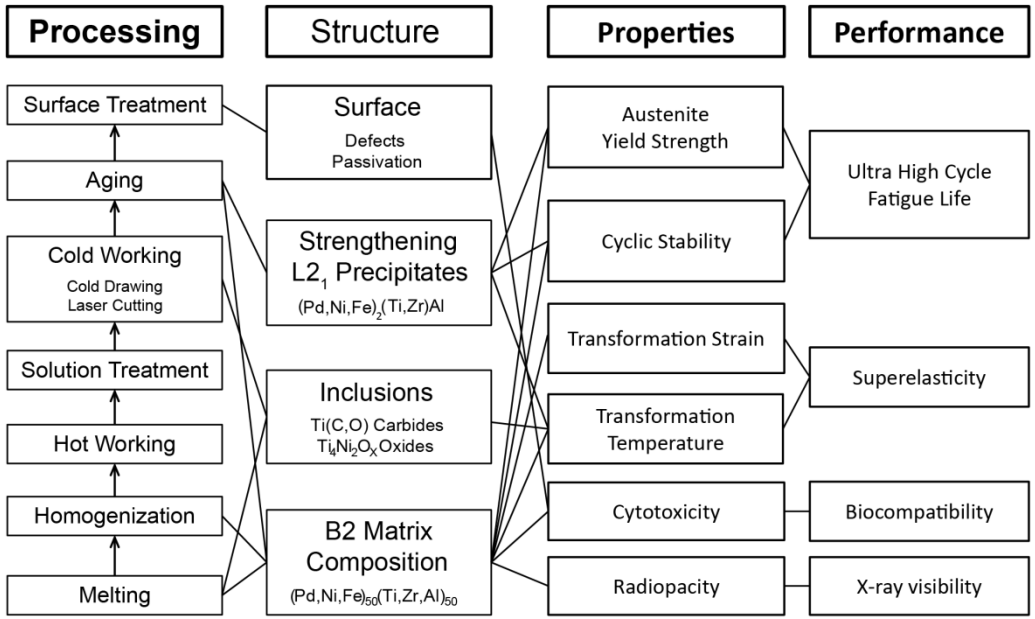


- Refined Co databases to match experiments
- Successfully reduced aging time (maintaining strength) using PrecipiCalc simulations, targeted experimentation
- Procured new heat of material (300-lb) for process optimization, data development for AIM calibration

PRECIPITATION-STRENGTHENED ALLOYS

DESIGN GOALS

- *Characterize phase relations, kinetics, and strengthening behavior in $L2_1$ Heusler strengthened low-Ni, high-strength "hybrid" (Pd,Ni)(Ti,Zr,Al) and Ni-free (Pd,Fe)(Ti,Al) alloy systems*
- *Demonstrate transformable hybrid alloy design and improve predictive transformation temperature model to allow for design of a superelastic hybrid alloy*



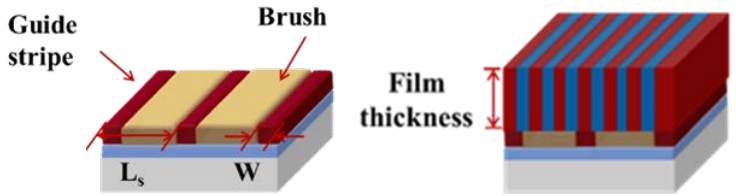
- A team of Northwestern undergraduates won 3rd place in ASM's Undergraduate Design Competition for their hybrid alloy design.
- A transformable low-Ni hybrid prototype was designed.
- The Ni-free alloy exhibited extremely high thermal cyclic stability and low hysteresis.
- FEA modeling that utilized an image-based mesh to predict minimum fatigue properties in the presence of an inclusion stringer.

USE-CASE GROUP

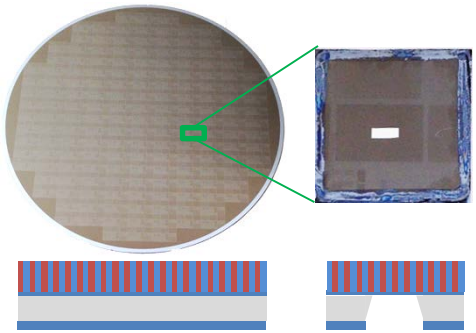
DIRECTED SELF-ASSEMBLY OF BLOCK COPOLYMERS

DESIGN GOALS

- *Materials and processes for sub 10 nm lithography*
- *Scaling to 5 nm resolution*



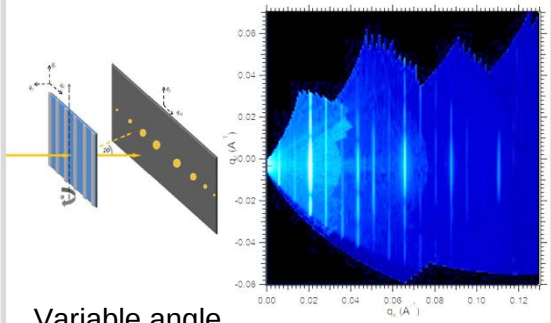
Relevant samples from industrial partners



300mm Wafer

Coupon with back-etched membrane

Resonant Soft X-ray Scattering (RSoXS)



Variable angle transmission measurement

Reconstruct Q_x-Q_z map

- Need to establish manufacturing-relevant materials and processes to realize sub 10 nm resolution, and scaling to 5 nm.
- Standard metrology cannot be used to develop and validate predictive models or prototypical systems.
- Objective: develop fully 3D metrology tools of DSA structures based on RSoXS
- Experiments are performed on samples fabricated by industrial partners
- Results are *quantitatively* compared with those of molecular simulations

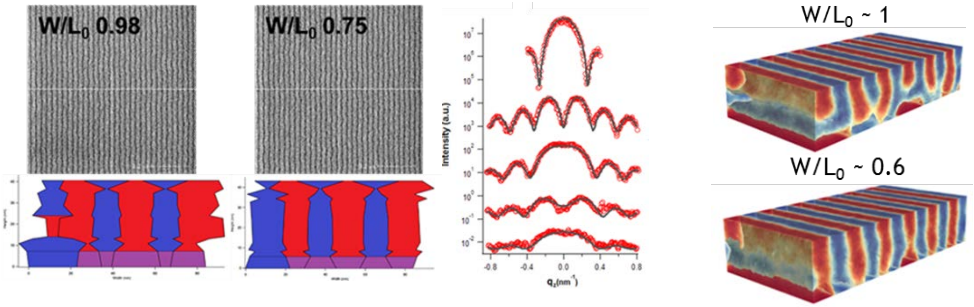
In-film structures revealed

Fit to experiment

Couple to molecular simulation

SEM

2D Model



NIST

CHiMaD

Governance

- **Directors**: Leadership, funding allocation, strategy
- **Executive Committee**: Monthly review, coordination, strategy
- **Technical Advisory Board**: External review, industry view
- **Use-Case Leads**: Leadership, foster engagement, outcomes
- **Cross-cut Leads:** Leadership, coordination, outcomes
- **Annual Meeting:** High-level review, engagement, TAB
- **Staff:** Logistics, Support, communication, progress

Significant Engagement

- NIST leveraging investment in MGI, $13.5M per year, and NIST leadership in interagency coordination (Locascio, Warren)
- In Chicago, 35 PI's, 27 Postdoctoral Fellows, 38 Graduate students
- At NIST, 37 staff, 20 Postdocs/Associates,
- 4 CHiMaD Postdoctoral Fellows, 2 On-site at NIST
- Multiple visits between sites; 1 PI sabbatical at NIST; NIST postdocs in Chicago (this week; 3 CHiMaD events)
- Summer undergraduate research program
- Monthly Executive Committee Meetings
- Annual Meeting

Joint Activities

- ASM Action in Education Committee, Materials Genome Toolset dissemination to materials UG programs
- Integration in Northwestern ICME MS program
- Interactions with Fayetteville State University
- Workshops with the community:
  - CALPHAD database development
  - Coarse graining in molecular systems
  - Materials Design
  - US-Japan: Materials Genome Initiative
  - Phase field methods Workshops (2)
  - Multivalent Interactions in Polyelectrolytes
- A MGI seminar series, jointly hosted by Northwestern University, University of Chicago, and Argonne National Laboratory

Benefits to NIST

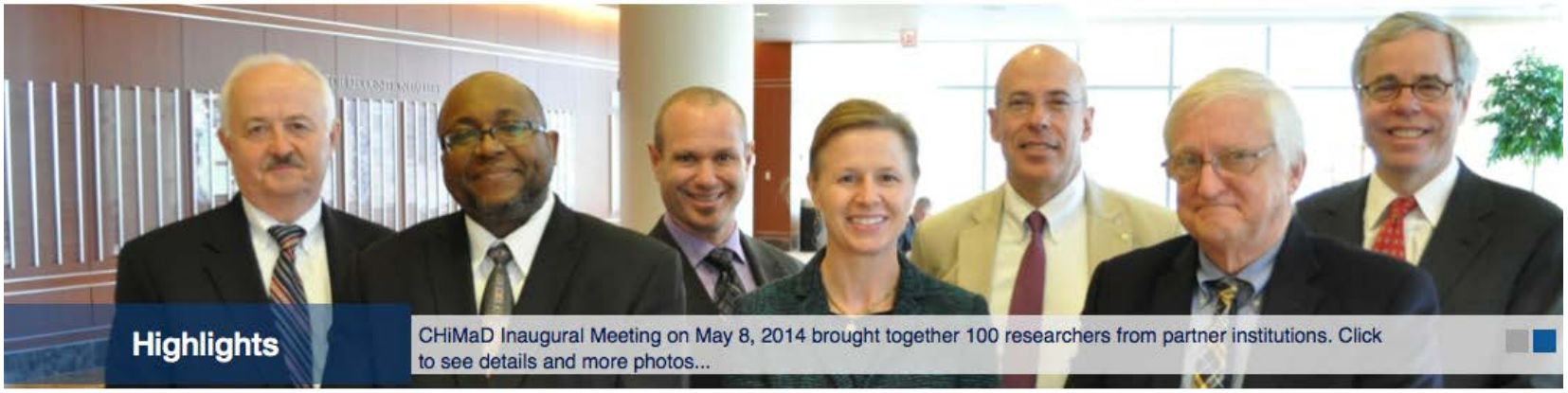
- Close partnership and access to concentration of world-class expertise in materials science
- Expansion of NIST expertise and capabilities, e.g. broaden and deepen technical depth, data (Globus), APS beamline
- Visible focus on MGI and advanced materials design for stakeholders
- Significant critical mass to effect changes in materials design, materials data, and advanced manufacturing

Lessons Learned / Challenges

- Extremely exciting, many unexpected new ideas and opportunities
- Building strong relationships takes time
- Coordination and communication around a shared vision are essential
- Critical mass in multiple areas needed to effect changes in materials design, materials data, and advanced manufacturing

Future Plans

- Building upon a strong foundation and start
- Continue integration into national MGI effort
- Focus on building and expanding communities around use cases, especially with a focus on industry engagement
- Develop framework for refreshing use-case areas into the future
- Continue focus on materials data and informatics tools



chimad.northwestern.edu

THANK YOU