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
USE-CASE GROUP

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

- 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
**USE-CASE GROUP**

**PRECIPITATION-STRENGTHENED ALLOYS**

**DESIGN GOALS**

- Characterize phase relations, kinetics, and strengthening behavior in L2₁ 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

In-film structures revealed

SEM

W/L₀ 0.98
W/L₀ 0.75

2D Model

Resonant Soft X-ray Scattering (RSoXS)

Variable angle transmission measurement
Reconstruct Qₓ-Q𝑧 map

Fit to experiment

Couple to molecular simulation

Guide stripe
Brush
Film thickness

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
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