Advanced Materials for Industry: NIST and the Materials Genome Initiative

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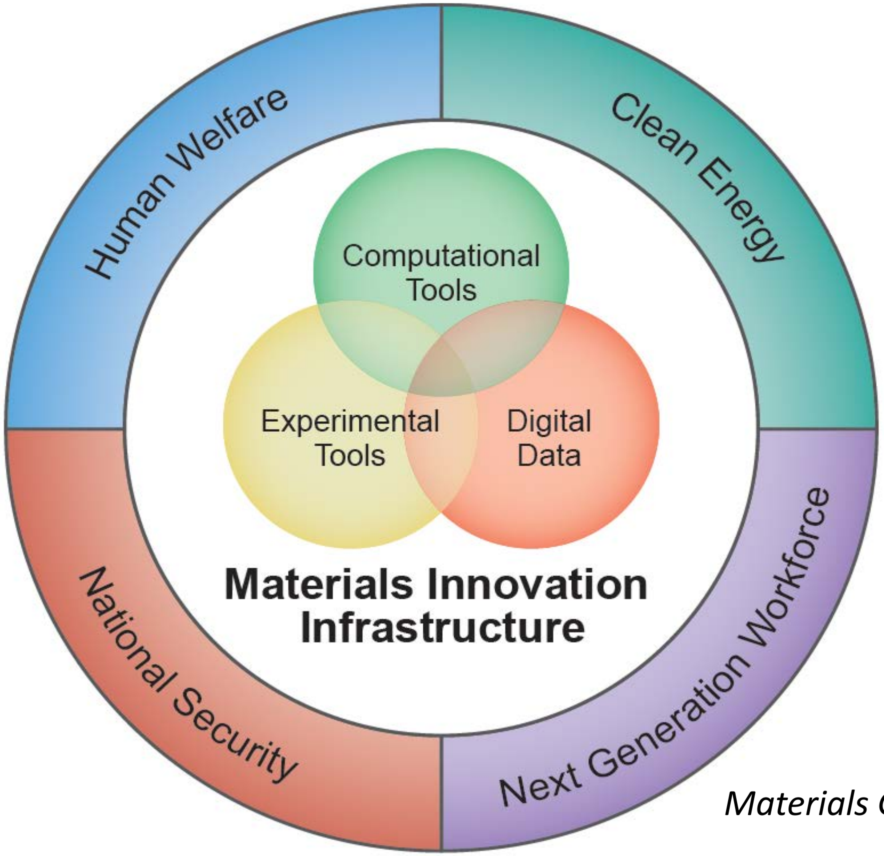
The Materials Genome Initiative

Goal: to decrease the cost and time-to-market by 50%

1. Develop a Materials Innovation Infrastructure

2. Achieve National goals in energy, security, and human welfare with advanced materials

3. Equip the next generation materials workforce



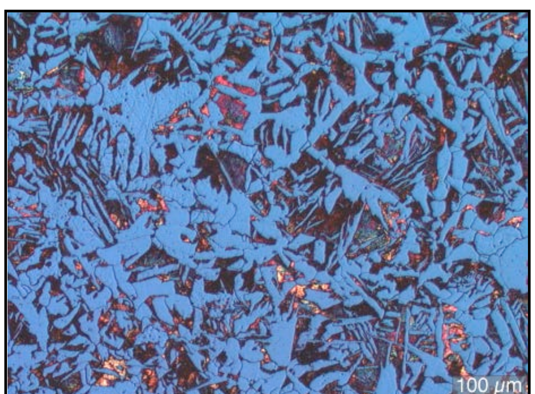
Materials Genome Initiative for Global Competitiveness

Why a Materials Genome Initiative?

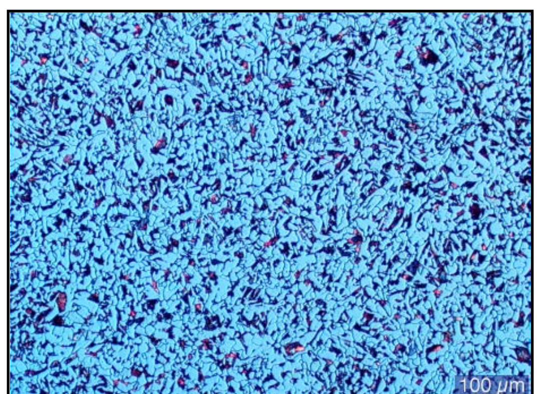
Materials Are Complicated Systems
Modeling is a Challenge

- Advanced materials are complex: multi-component and multi-phase
- Without adequate modeling, informatics and data exchange, the development of next generation materials using empirical approaches is bogged down by their complexity
- The Materials Genome Initiative seeks to advance materials design capabilities to promote faster, cheaper

Alloy cooled from 300 C



Alloy cooled from 800 C



- Composition and processing affect properties
- Phases change as a function of processing
- Microstructures consist of mixtures of multiple material phases
- Finer microstructure results in a much stronger alloy

FY12 NIST Budget Initiative: Advanced Materials For Industry

Provide the Measurement and Standards Infrastructure Needed to Realize the MGI

Implementation

NIST will work with stakeholders in industry, academia, and government to develop standards, tools and techniques for the

- Representation and interoperability of materials data, whether from simulation or experiment
- Interoperability of modeling systems on different scales
- Quality assessment of models, simulations, and materials data

Expected Outcomes

- Improved access to data/models/simulations
- Easier assembly of models that combine differing length and time scales
- Improved model reliability and confidence in results
- Reduced barriers to adopting state-of-the-art methods and techniques

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Pilot Projects in Advanced Materials Design

- Built upon existing NIST expertise in
  - Materials experimental analysis
  - Materials data
  - Software
- Initial pilot projects:
  - Structural metallic alloys of interest to, e.g. aerospace (superalloys) and transportation (lightweight alloys)
  - Advanced composites for application in transportation, energy, and electronics

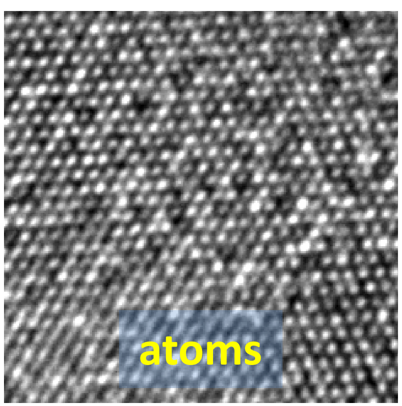
Pilot 1: Structural Metallic Alloys

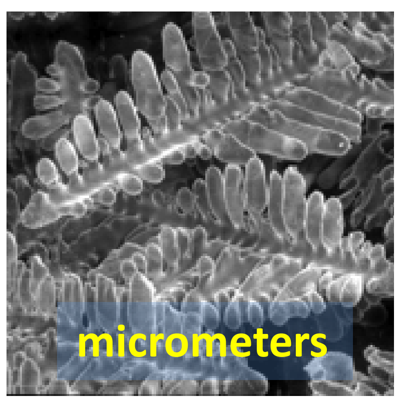
Processing creates the microstructure and microstructure establishes properties of material

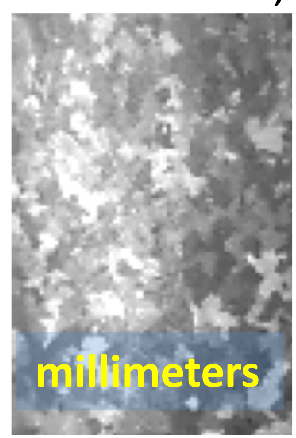
The pilot will allow us to start answering key questions including how to:

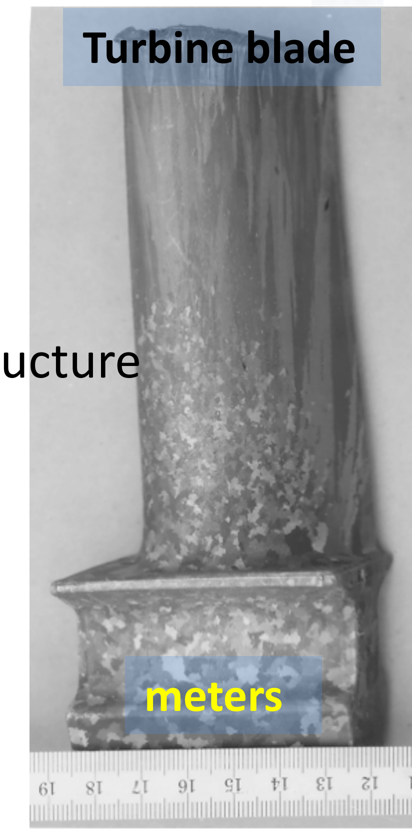
- make the physics-based model
- predict phases and phase distribution
- predict properties from the microstructure
- predict how the structure influences the material properties
- store and manage information

Application Areas: aerospace, automotive, structural steels, infrastructure









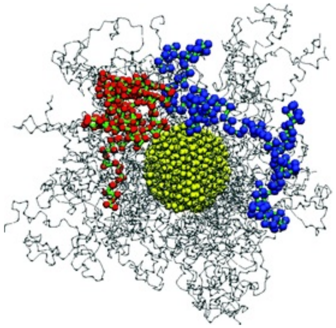
Pilot 2: Advanced Polymer Composites

Multi-scale dispersions of a solid phase in a polymer matrix, which exhibit strong dependencies between scales

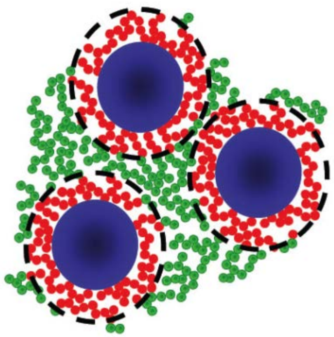
The pilot will allow us to start answering key questions including how to:

- predict bulk properties (e.g. yield strength, electrical, water diffusion)
- predict filler dispersion, orientation, localized mechanical properties
- predict fracture behavior, aging behavior
- enhance functionality (responsiveness, "smart materials")
- incorporate new concepts (nano-, sustainable)

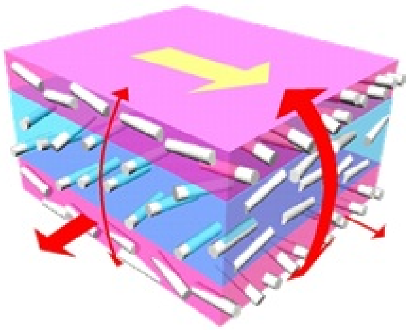
Application Areas: Lightweight replacements for metals, National security and law enforcement (e.g. helmets, body armor), sustainable and bio-based materials



Molecular Species
Courtesy: BASF



Interface & Dispersion
PRL, 98, 128302 (2007)



Laminate Structure
Courtesy: BASF

Revista Materia, 15(2), pp. 176-182, 2010.

Historical Success: Calculation of Phase Diagrams (CALPHAD)

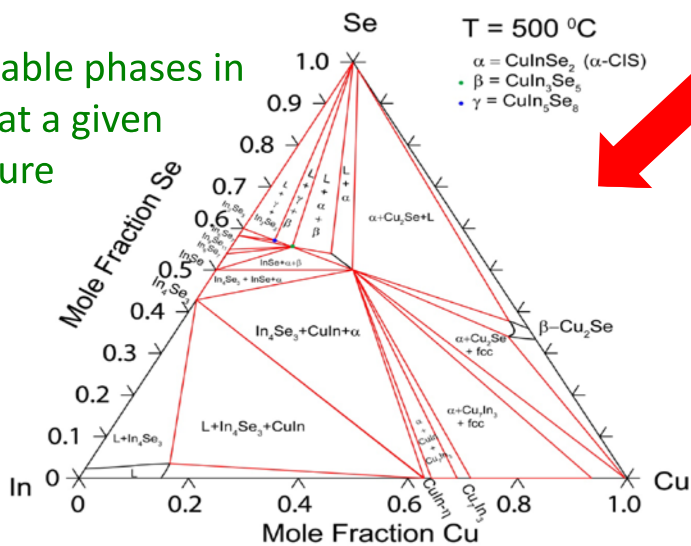
- Sparse Experimental Data
  - Phase equilibria
  - Thermodynamics
  - Diffusion
- Physics Based Models of Simpler Systems

Input

Parameter Optimization with CALPHAD (Computer Coupling of Phase Diagrams and thermochemistry)

- Enables extrapolation of higher order systems (multicomponent and multiphase) from binary and ternary systems

Map of stable phases in mixtures at a given temperature



Output

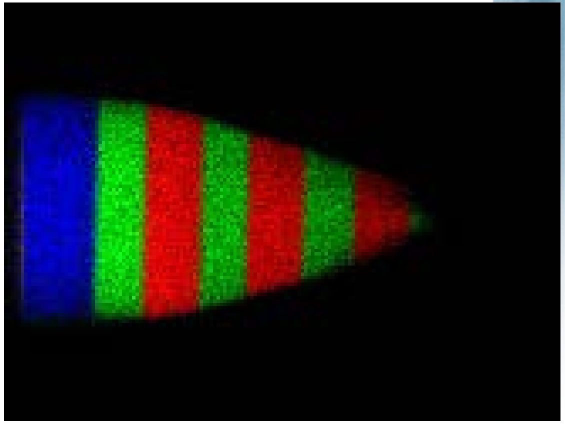
Rich models for choosing materials composition and designing processing routes

The CALPHAD method has been recently identified by the National Academies as "one of the pillars in Integrated Computational Materials Engineering"

MGI will change the way NIST does science and service

Leaps in Material Measurement Science

- MGI's Structural Models → *Powerful new tools for interpreting/mining data-rich materials images: tomography, hyper-spectral, atomic and chemical mapping…*
- MGI's Property/Structure Models → *Rational (rather than Edisonian) screening of discovery space and targeting of resource intensive materials characterization techniques: neutron, synchrotron, TEM…*



Ni-Cr Multilayer on Si
Mapped using hyperspectral x-ray energy dispersive spectroscopy

Next Generation Reference Material and Data Services

- MGI's Predictive Models → *Radically expand scope and depth of NIST SRDs: powerful tools for industrial materials selection and design*
- *MGI's Structure/Property Models → Accelerate development and deployment of niche SRMs for emerging materials technologies: improved support of innovation in energy, electronics, infrastructure, transportation…*

Recent Coordination Events

White House Event
The MGI: Catalyzing a National Movement

- Background: Started as a NIST workshop
- Goals: To kickoff the MGI on the national level and highlight new efforts in this area
- Some Outcomes:
  - 31 organizations signed on to the Orlando Materials Innovation Principles
  - 33 universities pledge to train materials workforce of the future
  - Multiple companies volunteered involvement and resources in areas such as data sharing, educational partnerships, and consortia

NIST Workshop
Building the Materials Innovation Infrastructure: Data and Standards

- Goals:
  - Initiate a conversation with leaders in materials community
  - Scope data/informatics challenges
- Some Outcomes
  - Identification of critical data/infrastructure challenges
  - Synthesize crosscutting data challenges across length scales
  - Develop Web 2.0 resources to enable collaborations
  - NIST follow on workshops (Fall 2012 – Uncertainty; Winter 2013- Model Interoperability)

Conclusions

- Nationally scoped program
- Broad stakeholder buy-in
- NIST mission defines a central role to realizing goals of initiative
- NIST MGI efforts builds off a strong, focused set of internal efforts

The hard work has already begun!

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