CHiMaD | Center for Hierarchical Materials Design

Peter Voorhees, Gregory Olson | *Northwestern University*
Juan De Pablo | *University of Chicago*

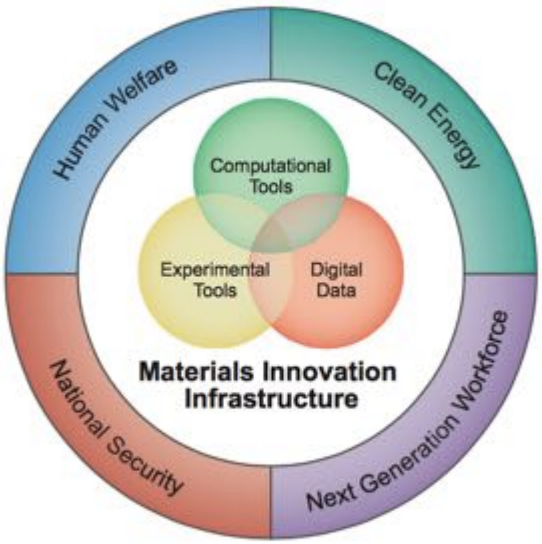
NIST

CHiMaD

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

- Developing a Materials Innovation Infrastructure
  - Integrated experimental, computational, and data informatics tools
  - Span entire materials continuum
  - Open-access/Open-source
- Achieving National Goals with Advanced Materials
  - Develop the *infrastructure* to design new materials
- Equipping Next Generation Materials Workforce
- Engaging all stakeholders
  - Government, academia, and industry



NIST Center for
Excellence in Advanced Materials

Center of Hierarchical Materials Design

THE UNIVERSITY OF CHICAGO

NORTHWESTERN UNIVERSITY

Argonne NATIONAL LABORATORY

QUESTEK INNOVATIONS LLC

ASM INTERNATIONAL

FAYETTEVILLE STATE UNIVERSITY

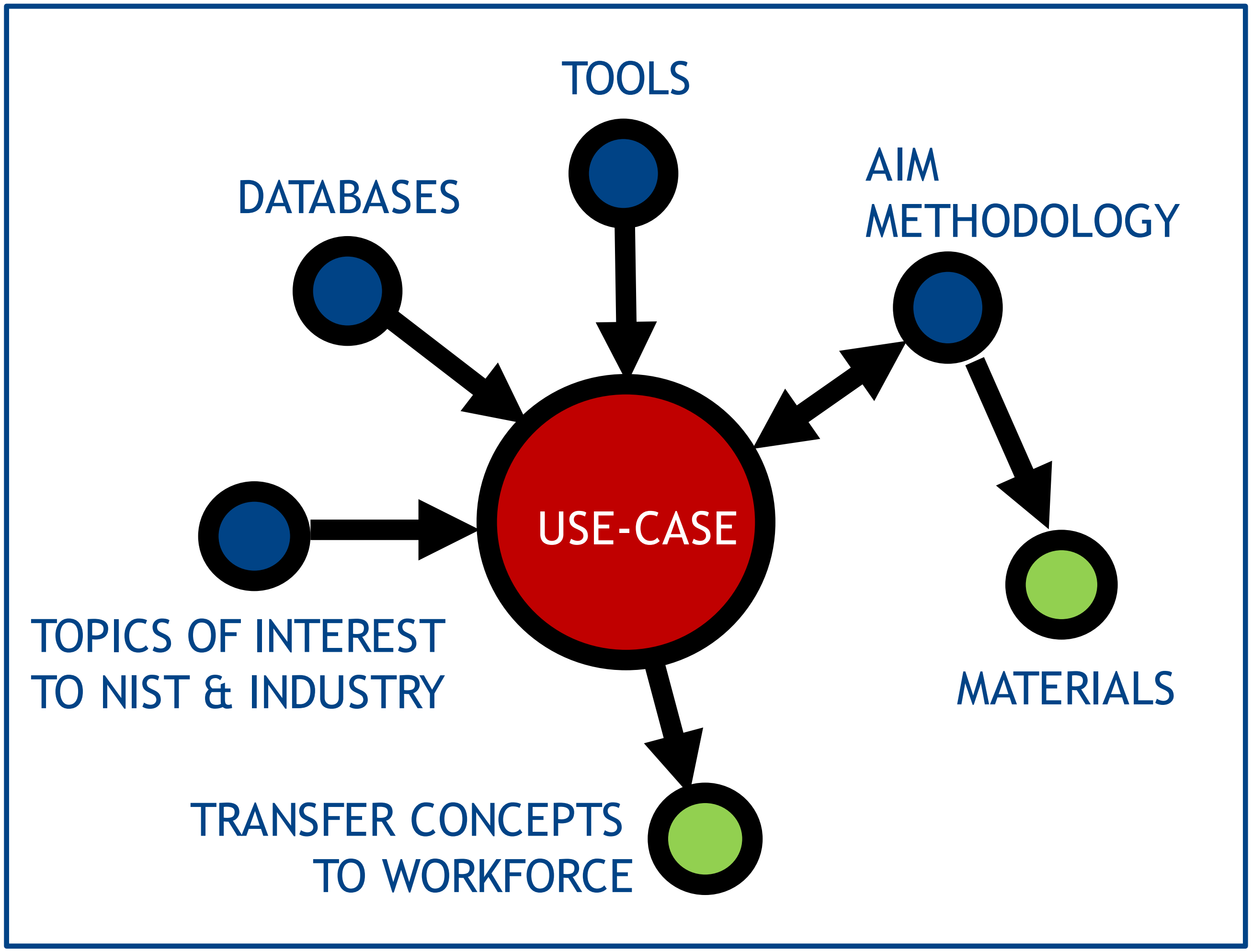
36 PIs | 34 Postdoctoral Fellows
38 Graduate Students | 40 NIST collaborators

CHiMaD

Objectives of CHiMaD

- *Create* a collaborative environment and concentration of scientific and technical capability to accelerate materials discovery and development
- *Provide opportunities* to transition new breakthroughs in advanced materials to industry
- *Convene* multidisciplinary and multi-sector communities for in-depth discussions
- *Provide training* opportunities for scientists and engineers in materials metrology
- *Foster* the development of integrated computation, modeling and data-driven tools
- *Foster* the discovery of new materials
- *Establish opportunities* for extended collaborations with NIST

Implementation



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Industrial Interactions: Technical Advisory Board

Many also participate as members of use-case groups

Industrial Participants

Dow
GM
ArcelorMittal
CATERPILLAR
Owens Corning
DMG MORI
GOODYEAR
Constellium

8

CHiMaD Use-Case Groups

- *Precipitation-Strengthened Alloys*
- *Low-dimensional Nanoelectronic Materials*
- *Data Mining*
- *Polymer Matrix Materials*
- *Directed Self-Assembly of Block Copolymers Films for Lithographic Applications*
- *Soft Matter Design based on Charge Complexation*
- *Organic Bulk Heterjunction Polymer Solar Cells*
- *In Situ Si-Composites*

Seed Groups & Other Efforts

- *Additive Manufacturing*
- *Phase Field Methods*
- *Coarse-grained simulations of OPVs*
- *Data/Databases*
- *Materials Data Facility*
- *Thermoelectrics*
- *Impact Mitigation*
- *Materials Research Facility*

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CHIMAD USE-CASE GROUPS

All use-case and tool groups have significant NIST participation

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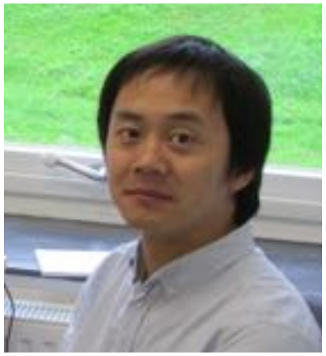
Fanny Rodolakis-Simoes

Nana Ofori-Opoku



Peisheng Wang

Marat Andreev

NIST-CHIMAD POSTDOCS

CHiMaD

Steve Davis, NU

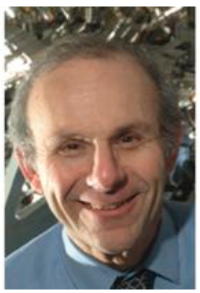
Peter Voorhees, NU

Wing-Kam Liu, NU

Christopher Wolverton, NU

Jason Sebastian, Questek

Alexander Umantsev, FSU



David Seidman, NU

Alok Choudhary, NU

Wei Chen, NU

Ankit Agrawal, NU

Yip NU

NIST Collaborators

Carelyn Campbell
Ursula Kattner
Eric Lass
Kil-Won Moon
Maureen Williams

Gregory Olson, NU

David Dunand, NU

PRECIPITATION-STRENGTHENED

predictive design of precipitation-st being applied to Co-based superalloy shape-memory alloys

Constellium

QuesTek INNOVATIONS LLC

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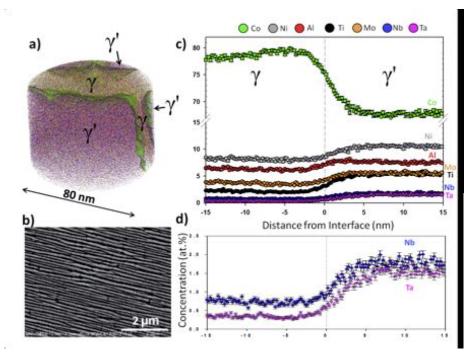
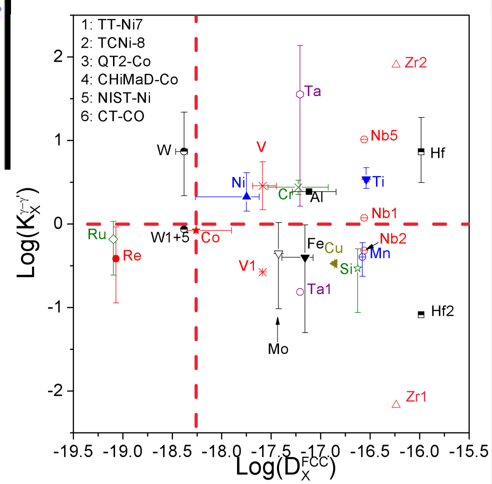
PRECIPITATION-STRENGTHENED ALLOYS: Co-based

DESIGN GOALS

- *Near-term: Apply accelerated insertion of materials (AIM) approach for accelerated qualification of precipitation-strengthened Co-based bushing/actuator alloy use case*
- *Longer-term: Apply computational design to high-temperature Co alloys*



New 300# VIM/VAR heat
QT-Co homogenized
& hot forged

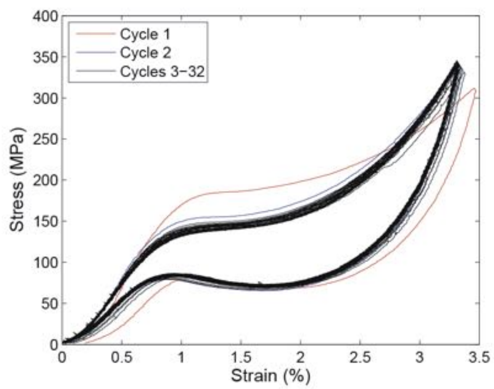


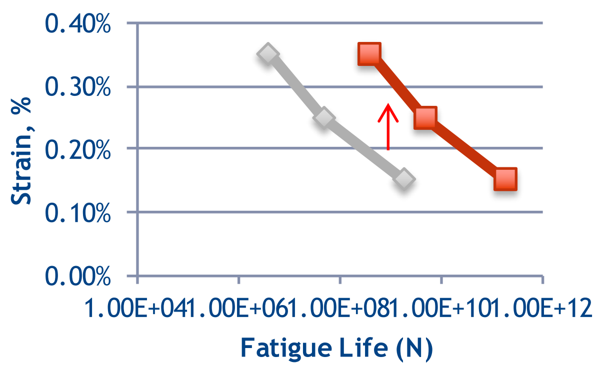
- Continued refinement of Co thermodynamic and mobility databases in NIST collaboration.
- Procured new 300-lb VIM/VAR heat of QT-Co bushing alloy, refined homogenization and forging conditions for completion of thermal process optimization; new QT SBIR obtained to aid AIM qualification.
- Detailed microanalysis of experimental alloys quantify phase relations for high-temperature alloys and populate pre-CALPHAD data.
- Search cross-plot of fundamental data prioritizes new components for high-throughput experiment and theory, supporting expanded CALPHAD assessment

PRECIPITATION-STRENGTHENED ALLOYS: SMAs

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 for SMA design with enhanced cyclic stability.*
- *Employ FEA simulation of fatigue nucleation to predictively optimize inclusion distribution for enhanced minimum UHCF fatigue performance.*





-Completed doctoral thesis of Dr.Dana Frankel (MSE) demonstrated superelastic peak-strengthened Ni-free alloy with high thermal cyclic stability and low hysteresis. Transformable low-Ni Pd-Zr hybrid prototype calibrated role of misfit in strengthening efficiency.

-FEA modeling performed in student team collaboration with Dr. John Moore (ME) used an image-based mesh to predict 2X minimum UHCF fatigue property improvement with 3X inclusion size refinement.

NIST Collaborators

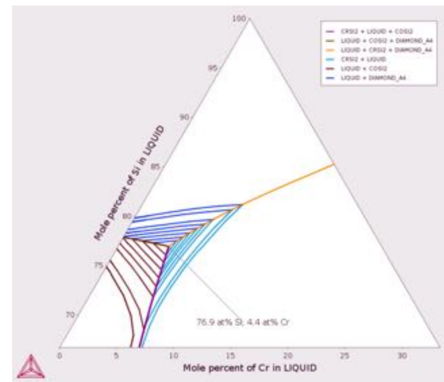
James Warren
Ursula Kattner

Dow-Corning Collaborators

Vasgen Shamamian
Kwon Skinner
Andreas Becerra
Lance Wu

Peter Voorhees, NU

Christopher Wolverton, NU



IN-SITU SI COMPOSITES

using computations, verified databases, and experiments, in collaboration with Dow Corning, to design high performance Si-based composite materials for structural applications which are both tough and melt castable. The focus of the use-case group is on Si-Cr-Ti-Co alloys.

DOW CORNING

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In-situ Si Composites

- Vasgen Shamamian (Dow-Corning),
- Kwon Skinner (Dow-Corning),
- Andres Becerra (Dow-Corning),
- Lance Wu (Dow-Corning)
- James Warren, Ursula Kattner (NIST)
- Kwon Skinner was located at Northwestern part time
- Northwestern team visited Dow Corning
- NIST Postdoc spends 3 months a year at CHiMaD
- CHiMaD student spent 2-3 weeks at NIST
- Met every two weeks with Dow-Corning

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Interactions with Dow-Corning

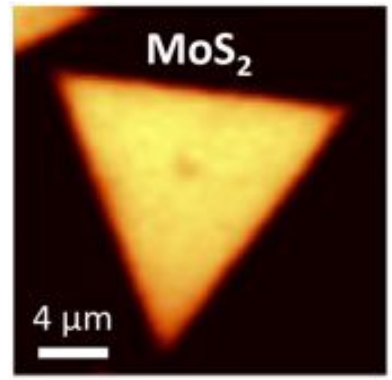
- An accurate description of phase equilibria in the Si-Cr-Ti system is needed
- In collaboration with NIST, Matt Peters produced an assessment using publically available data
- Dow-Corning then augmented this dataset with their proprietary data
- This data was used to design alloys that avoid cracking on solidification
- Last year a new Chief Technical Officer was hired and the program was cancelled

NIST Collaborators

Albert Davydov
Francesca Tavazza
Arunima Singh
Sergiy Krylyuk

Mark Hersam, NU

Lincoln Lauhon, NU



2D HETEROSTRUCTURES FOR ELECTRONICS

to understand and realize p-type and n-type doping in the low-dimensional limit. The interplay between experiment and computation accelerates the understanding and design of doped low-dimensional nanoelectronic materials and their heterostructures.

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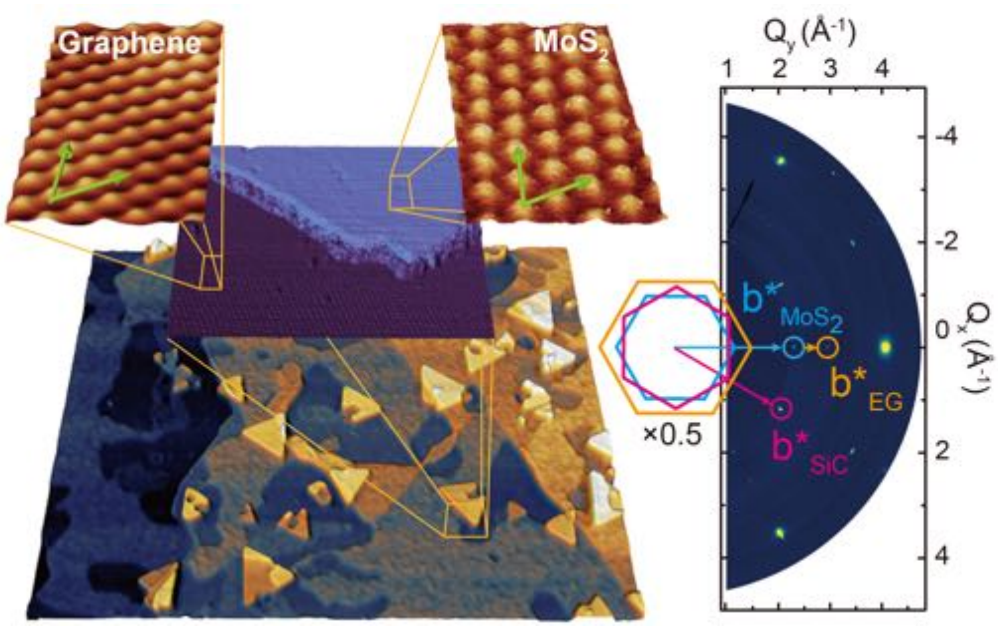
USE-CASE GROUP

M. HERSAM, NU

LOW-DIMENSIONAL NANOELECTRONIC MATERIALS

DESIGN GOALS

- *Control Doping and Carrier Concentration in Low-Dimensional Semiconductors*
- *Develop Heterostructures Consisting of Low-Dimensional Nanoelectronic Materials*



Atomically resolved scanning probe microscopy and synchrotron X-ray scattering reveal rotational commensurability in MoS_2/graphene heterostructures.

- MoS_2/graphene heterostructures have been realized by chemical vapor deposition.
- The van der Waals interactions between MoS_2 and epitaxial graphene on SiC lead to rotationally commensurate growth.
- Rotational commensurability implies exceptionally low defect density and significantly reduced angular distribution for grain boundaries.
- The improved crystal quality has positive implications for electronic/optoelectronic properties and applications.

Hersam, Bedyzk, *et al.*, *ACS Nano*, **10**, 1067 (2016).

CHIMaD

Paul Nealey,
UChicago

Juan de Pablo,
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Steven Sibener,
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Luping Yu,
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Ian Foster,
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NIST Collaborators

Joseph Kline
Debra Audus
Jack Douglas
Daniel Sunday
Jonathan Winterstein
Alexander Liddel
Adam Hannon
Kenneth Kronlein

DIRECTED SELF-ASSEMBLY OF BLOCK COPOLYMERS

to revolutionize nanomanufacturing. the interest and exponential growth in research activity and expenditure is driven by the semiconductor industry.

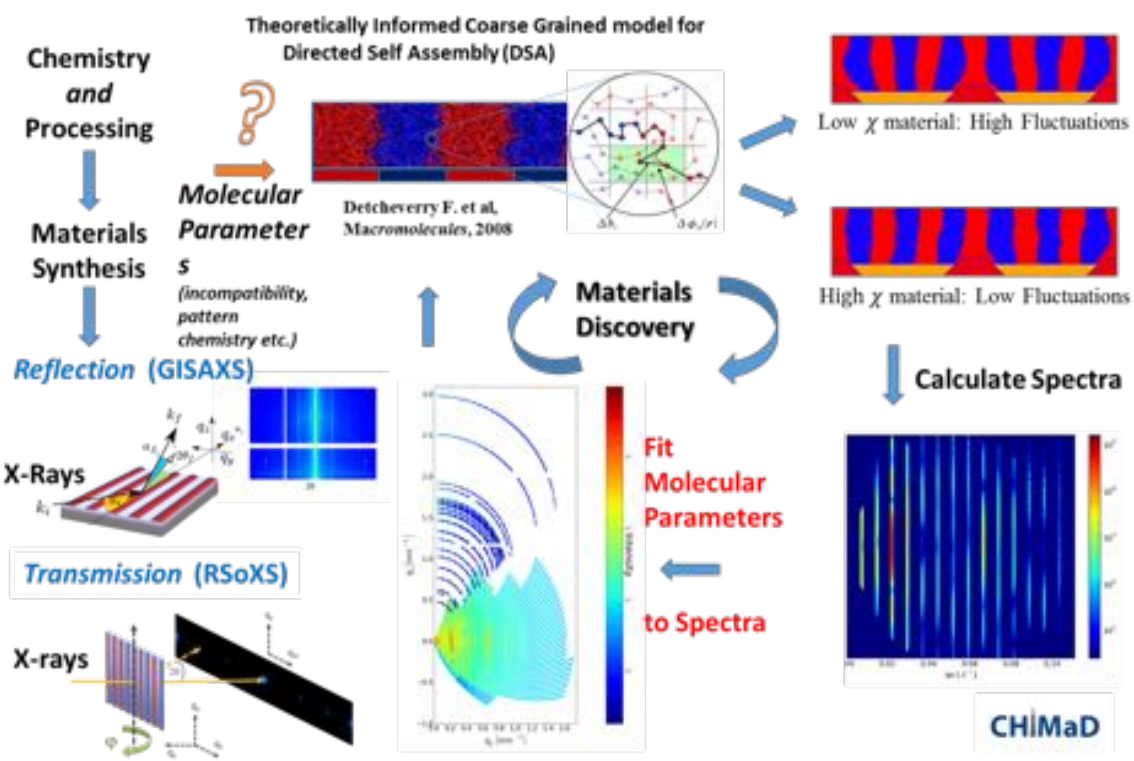
USE-CASE GROUP P. NEALEY, UCHICAGO

DIRECTED SELF-ASSEMBLY OF BLOCK COPOLYMERS

DESIGN GOALS

- *Materials and processes for sub 10 nm lithography, Scaling to 5 nm resolution - Lines and spaces*
- *Meet manufacturing constraints (Defects (.01/cm²); CD uniformity, LER/LWR (<1 nm)*
- *Beyond structure-property relationships - Dynamics of DSA systems and the impact on defectivity*
- *Self-aligned DSA of multi-color manufacturing-relevant patterns using triblock copolymers*

Experiments with ultra-high information content ↔ **Develop and validate predictive models of materials and processes**



- Physics-based model
- Inputs: >20 process and material parameters
- Solved using evolutionary algorithms
- Outputs:
- Simultaneous optimization of process and material properties towards design goals
- Material properties – many of which cannot be measured directly
- Quantitative fully three-dimensional structure

A new MGI paradigm for developing hierarchical mesoscale structures and processes

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Catherine Brinson, NU

Wei Chen, NU

NIST Collaborators

Chelsea Davis
Jeffrey Gilman
Jack Douglas
Frederick Phelan
Ketan Khare
Douglas Fox
Jeremiah Woodcock

Sinan Keten, NU

Juan De Pablo, UChicago

Erik Luijten, NU

POLYMER MATRIX COMPOSITES

to develop a "materials informatics initiative" including integrated databases, curation, visualization, and analysis tools to relate macroscale polymer composite behavior to chemical constituent and kinetic behavior, and linking these resources to further development of high-performance modeling and predictive tools

OWENS CORNING

GOODYEAR

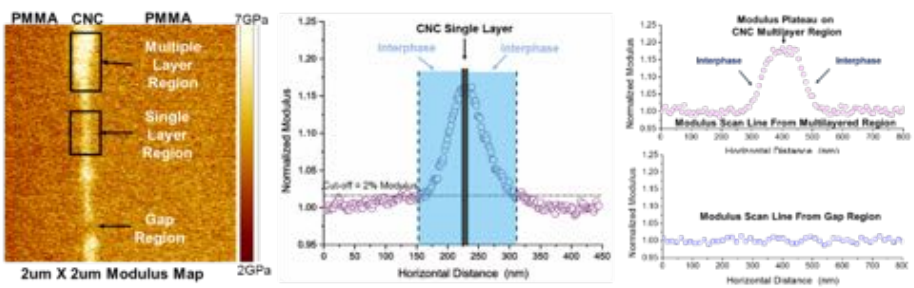
CHiMaD

POLYMER MATRIX MATERIALS

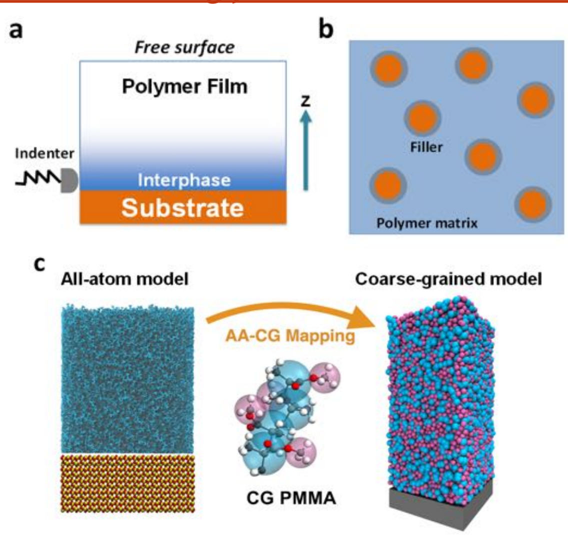
DESIGN GOALS

- *Develop design rules to tune the properties and service life of polymer matrix composites*
- *Manipulate and tune the interphase and the resultant bulk materials properties of nanocellulose-polymer nanocomposites utilizing databases, models, and experimental tools.*

Experiments to quantify interphase properties

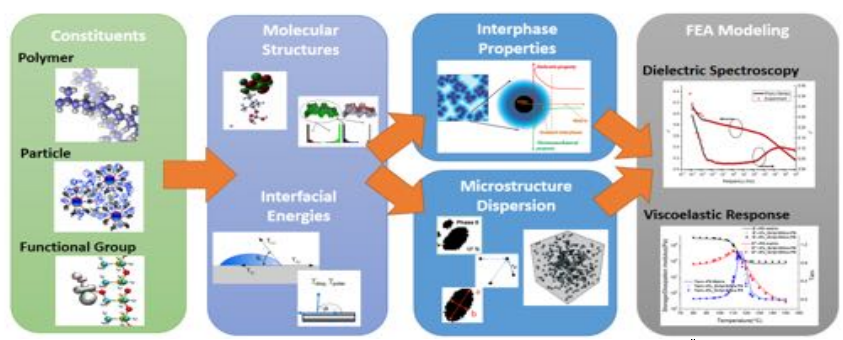


Multiscale modeling for nanoscale and bulk properties



- Data-driven modeling of processing & interfacial energies -> microstructure dispersion
- Integration of multi-scale modeling and experimental efforts to investigate local property gradient at interphase
- Nanocomposite data resource built with NIST Material Data Curator (NanoMine) with predictive analysis and modeling
- Collaborations and interactions for nanocomposite characterization (e.g. Owens Corning, NIMS)

Data resource, data-driven modeling and material design



NIST Collaborator
Lee Richter

Luping Yu, UChicago

Juan de Pablo, UChicago

Giulia Galli, UChicago

Tobin Marks, NU

ORGANIC BULK HETEROJUNCTION POLYMER SOLAR CELLS

bulk heterojunction organic solar cells (OSCs) represent an alternative solar energy harvesting system. New polymers and theoretical methods developed will deepen our understanding in structure/property relationship and push the performance of OSCs towards commercial applications.

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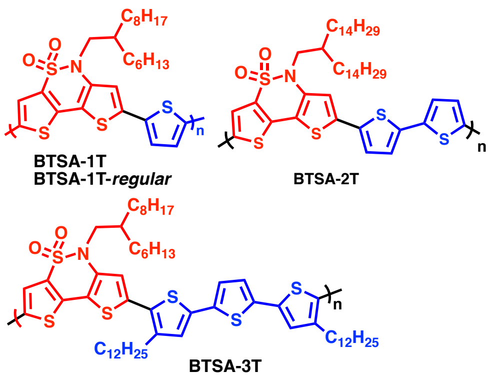
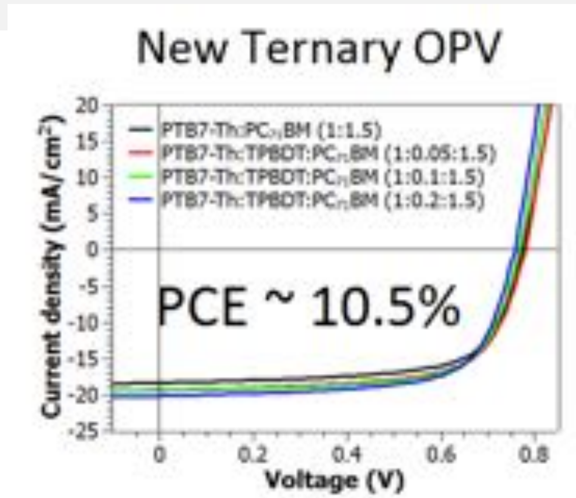
ORGANIC BULK HETEROJUNCTION POLYMER SOLAR CELLS

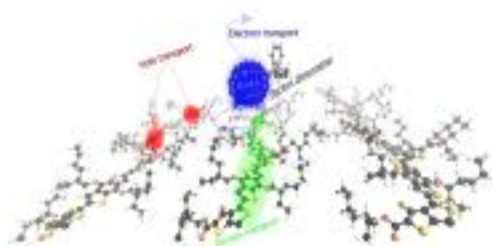
DESIGN GOALS

Apply MGI principles to critical issues in structure/function and processing/structure relationships to accelerate OPV device development.

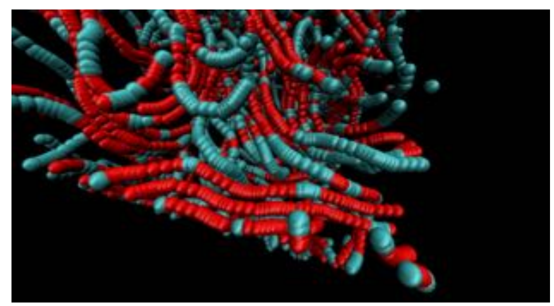


New Second Generation Building Blocks

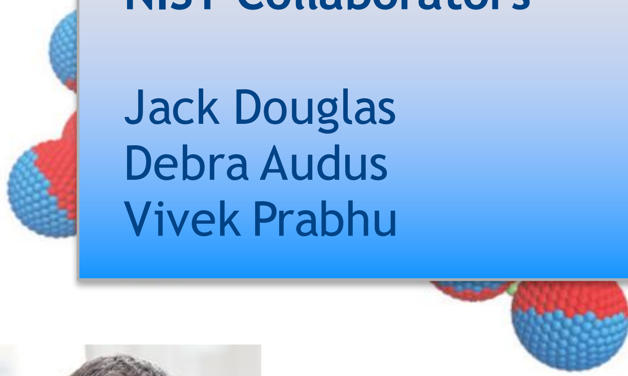




Electronic structure properties



Molecular dynamic simulation of new Bulk PTB7



NIST Collaborators

Jack Douglas
Debra Audus
Vivek Prabhu

Matthew Tirrell, UChicago

Juan de Pablo, UChicago

Monica Olvera de la Cruz, NU

Erik Luijten, NU

SOFT MATTER DESIGN BASED ON CHARGE COMPLEXATION

to develop new materials based on multi-valent ionic interactions. This can yield new types of self-assembled structures. Knowledge of the as-yet unexplored phase behavior of polyelectrolyte complexes is scientifically significant and technologically relevant.

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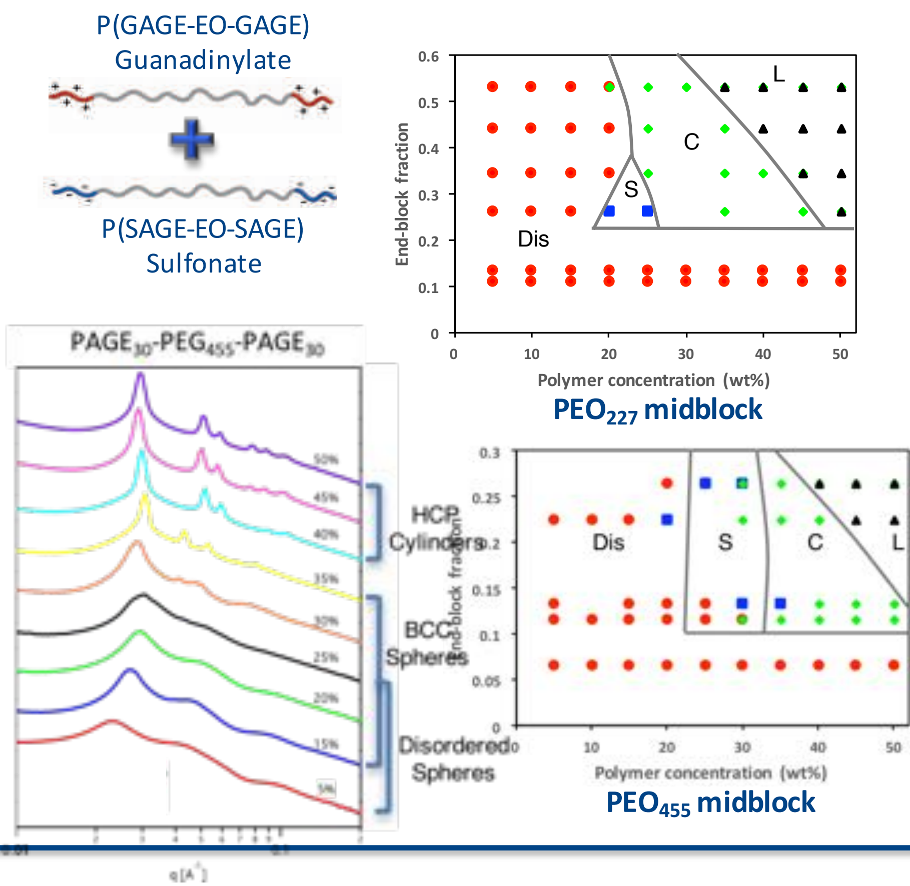
SOFT MATTER DESIGN BASED ON CHARGE COMPLEXATION

DESIGN GOALS

- *Control hydrogel bulk structure by varying lengths of molecular constituents and polymer loading*
- *Tune hydrogel sensitivity to salt and pH by varying block lengths, based on advances in reliable experimental phase diagrams and predictive theory*
- *Combination of salt, pH and macromolecular structure gives tunable moduli*
- *Extension to polypeptide materials with desired biocompatibility and biodegradability envisioned*



- Electrostatically cross-linked hydrogels obtained from mixing aqueous solutions of A_+BA_+ and $A\_BA\_$ triblock copolymers
- Polyelectrolyte complex (PEC) domains serve as tunable cross-links
- The ratio of charged:neutral block size determines
  - ❑ Size and spacing of the PEC domains
  - ❑ Aggregation number
- PEC morphology varies with polymer loading
- Morphology phase diagram in excellent agreement with the SCFT predictions
- Combining block size ratio and polymer loading variations allow for tunable mechanical properties

Alok Choudhary, NU

Ankit Agrawal, NU

Gregory Olson, NU

Christopher Wolverton, NU

Wei Chen, NU

NIST Collaborators

Alden Dima
Kenneth Kronlein
Adele Peskin
Sarala Padi

DATA MINING

To make significant advances in data-driven informatics to accelerate materials discovery

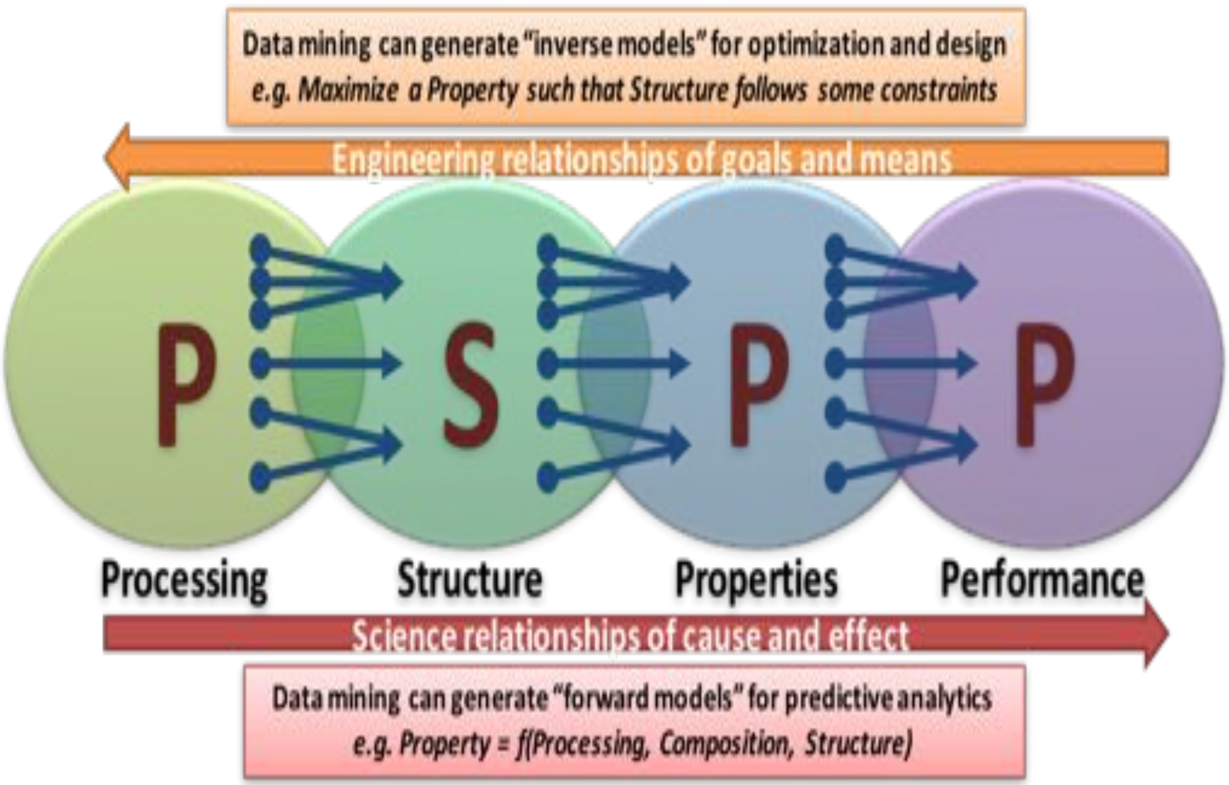
CHiMaD

A. CHOUDHARY, A. AGRAWAL, NU

DATA MINING

GOALS

- *Developing data-driven informatics to accelerate materials discovery and design*
- *Extracting actionable insights at unprecedented latency via bottom-up and hypothesis-driven discoveries*
- *Data mining on various heterogeneous and big databases that are complex, high dimensional, structured and semi-structured*



Research Accomplishments and Ongoing Efforts

- Integrating CALPHAD and Data Mining for Advanced Steel Design
- Composition-based Machine Learning Framework for Predicting Inorganic Material Properties
- Supervised Learning-based Microstructure Characterization and Reconstruction
- Fast Models for Properties of Crystalline Compounds Using Voronoi Tessellations and Machine Learning
- Classification of Scientific Journal Articles to Support NIST Data Curation Efforts
- Towards Designing OPV devices using Data Mining

E. Begum Gulsoy
Associate Director & Outreach

OUTREACH

Towards a resource for the community

CHiMaD

ASM Materials Genome Toolkit

- Toolkit includes main materials design software: *ThermoCalc*, *DICTRA*, *PRISMA*
- Awarded 7 schools with the toolkit in 2015; awarded schools took ***1st***, ***2nd***, ***3rd*** place at *2015 ASM Undergraduate Design Competition*

Outreach activities

- Phase Field Methods Workshop I-II & Hackathon
- Materials Design Workshop I-II
- Semi-automated Database Creation course (UC)
- Scientific Symposium on Multivalent Interactions in Polyelectrolytes
- Advances & Challenges in Soft Photovoltaic Research
- SRG Meeting

MGI Seminar Series

15 Seminars by international colleagues, broadcast live to CHiMaD institutions

Outreach to underrepresented groups

- Broadcast MAT 390: Materials Design (Olson) to FSU
- Negotiated a full 3-year Toolkit license for FSU, at no-cost to FSU
- Nana Ofori-Opoku gave a seminar at FSU
- (2016 Summer) UC Summer Course in collaboration with *Chicago Collegiate Scholars Program*
- (2016 Summer) Student sponsored under NU-MRSEC REU program, working on CHiMaD project

CHiMaD

Laura Bartolo
NAISE

Databases

TOOL DEVELOPMENT

Addressing the no data and the big data challenges

CHIMaD

CALPHAD Protodata Databases

Gregory Olson, NU

Peter Voorhees, NU

Christopher Wolverton, NU

- Tie lines, thermochemical data, elastic constants, Unlike assessed CALPHAD databases, which can be proprietary, this will be open
- Si, Co, and low Ni-SMA alloy systems
- NIST Data Curator

TOOL DEVELOPMENT
DATABASES

NanoMine

Catherine Brinson, NU

Wei Chen, NU

processing, structure and property parameters for polymer nanocomposite systems

http://nanomine.northwestern.edu:8000

Polymer Design

Juan de Pablo, UChicago

Ian Foster, UChicago

Paul Nealey, UChicago

Heinrich Jaeger, UChicago

characteristic properties for design of polymer blends and copolymers for engineering applications

ACS very supportive of our effort and is interested in collaborating

TOOL DEVELOPMENT

DATABASES

MATERIALS DATA FACILITY

Ian Foster, UChicago

- Objectives:
  - *publish* data to MDF storage, along with associated metadata
  - *discover* interesting data
  - *access* the data (and analysis and display where needed)
- The Facility:
  - allows users to share the *large* datasets
  - has cloud-hosted publication and discovery services
  - employs high-performance physical storage
  - Uploaded 10 TB of 4D tomographic data
  - https://materialsdatafacility.org

Software and Experimental Tools

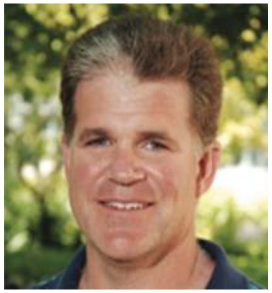
TOOL DEVELOPMENT

Community-Standard Phase Field Methods

Peter Voorhees, NU

Olle Heinonen, ANL

Barry Smith, ANL



David Chopp NU

NIST Collaborators

James Warren
Jonathan Guyer

Key computational method, but needs to be utilized as a materials design tool

Phase Field Methods Workshop I – Jan 9
Phase Field Methods Hackathon – Oct 14
Phase Field Methods Workshop II – Oct-15/16
Workshop III & Hackathon – May 3-5

Alexander Umantsev FSU

Fatigue Modeling using Phase Field Methods

TOOL DEVELOPMENT SOFTWARE

CHiMaD

Rapid Assessment of Phase Relations

Michael Bedzyk, NU

Yip-Wah Chung, NU

will develop the thermodynamic and mobility database for the highest priority alloying elements

Resonant Soft X-Ray Scattering

Paul Nealey, UChicago

will allow to follow evolution of polymer nanostructures for the directed self-assembly

TOOL DEVELOPMENT
EXPERIMENTAL

CHiMaD

Coarse Grained Simulations for OPVs

Monica Olvera de la Cruz, NU

Additive Manufacturing

Jian Cao, NU

Impact Mitigation

Sid Nagel, UChicago

Heinrich Jaeger, UChicago

Juan de Pablo, UChicago

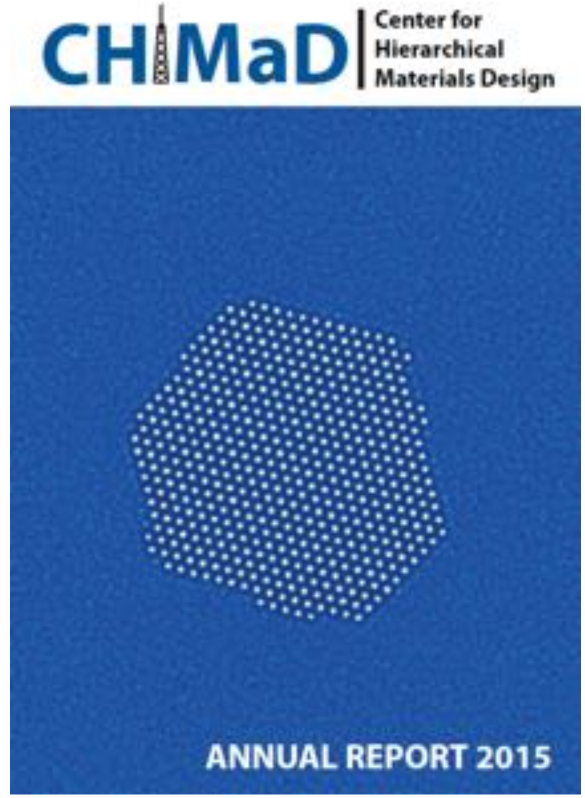
Seed Groups

CHiMaD

A Few Metrics

After 1.5 years of funding:

2015	2016	
10	42	Publications by CHiMaD researchers, accepted or published. (Does not include Use-Case group, NIST only publications)
71	145	Presentations delivered by CHiMaD researchers
18	40	NIST Collaborators
10	15	MGI Seminars hosted
1	3	PIs that spent time at NIST for research purposes. (Does not include workshops)



chimad.northwestern.edu

THANK YOU

CHiMaD