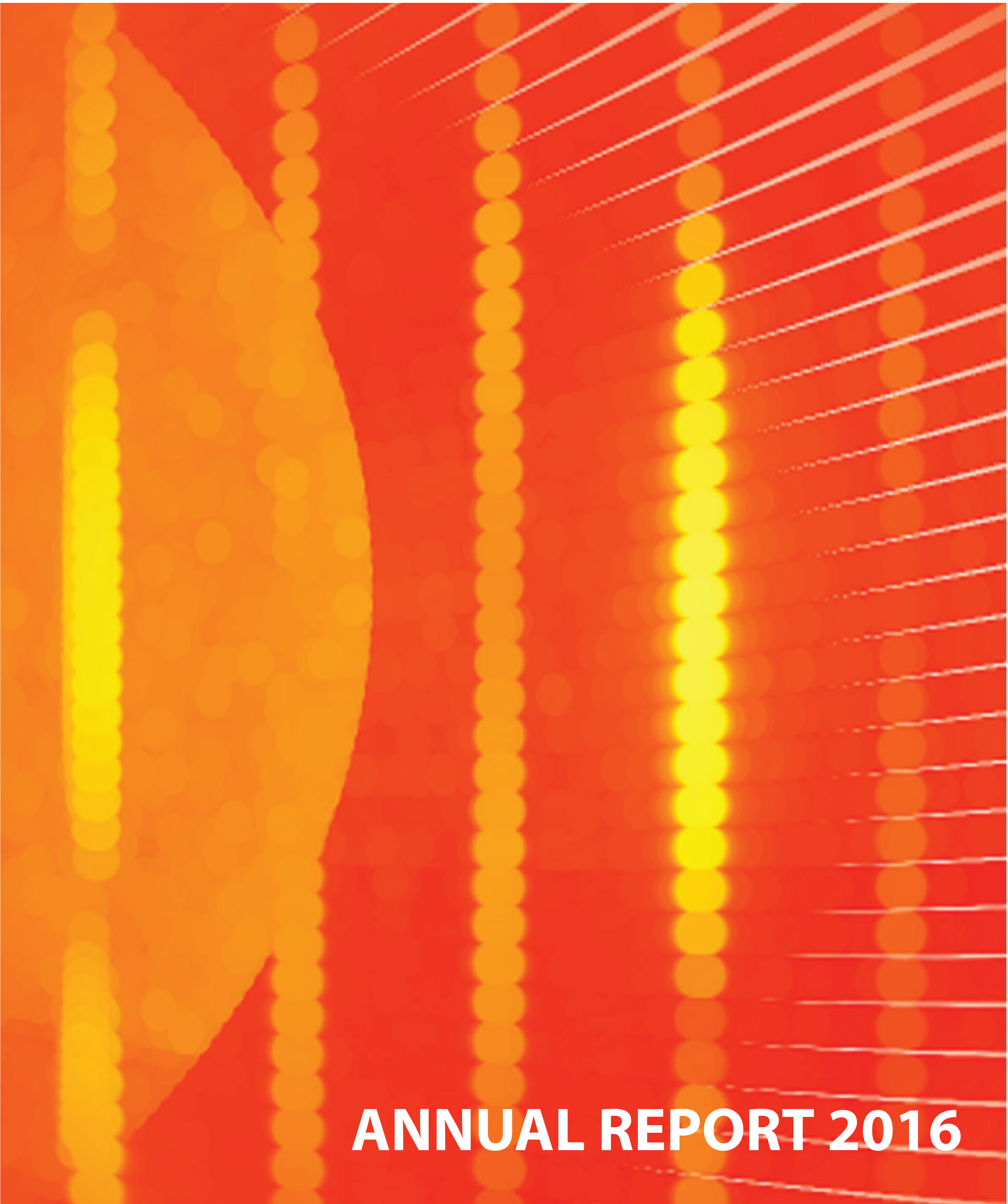
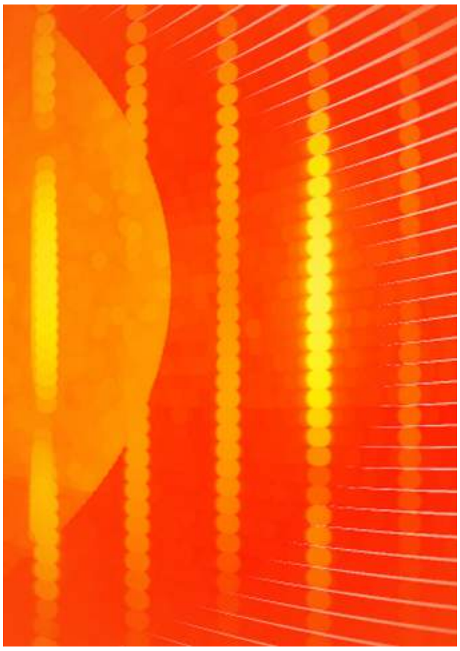
CHiMaD

Center for
Hierarchical
Materials Design



ANNUAL REPORT 2016



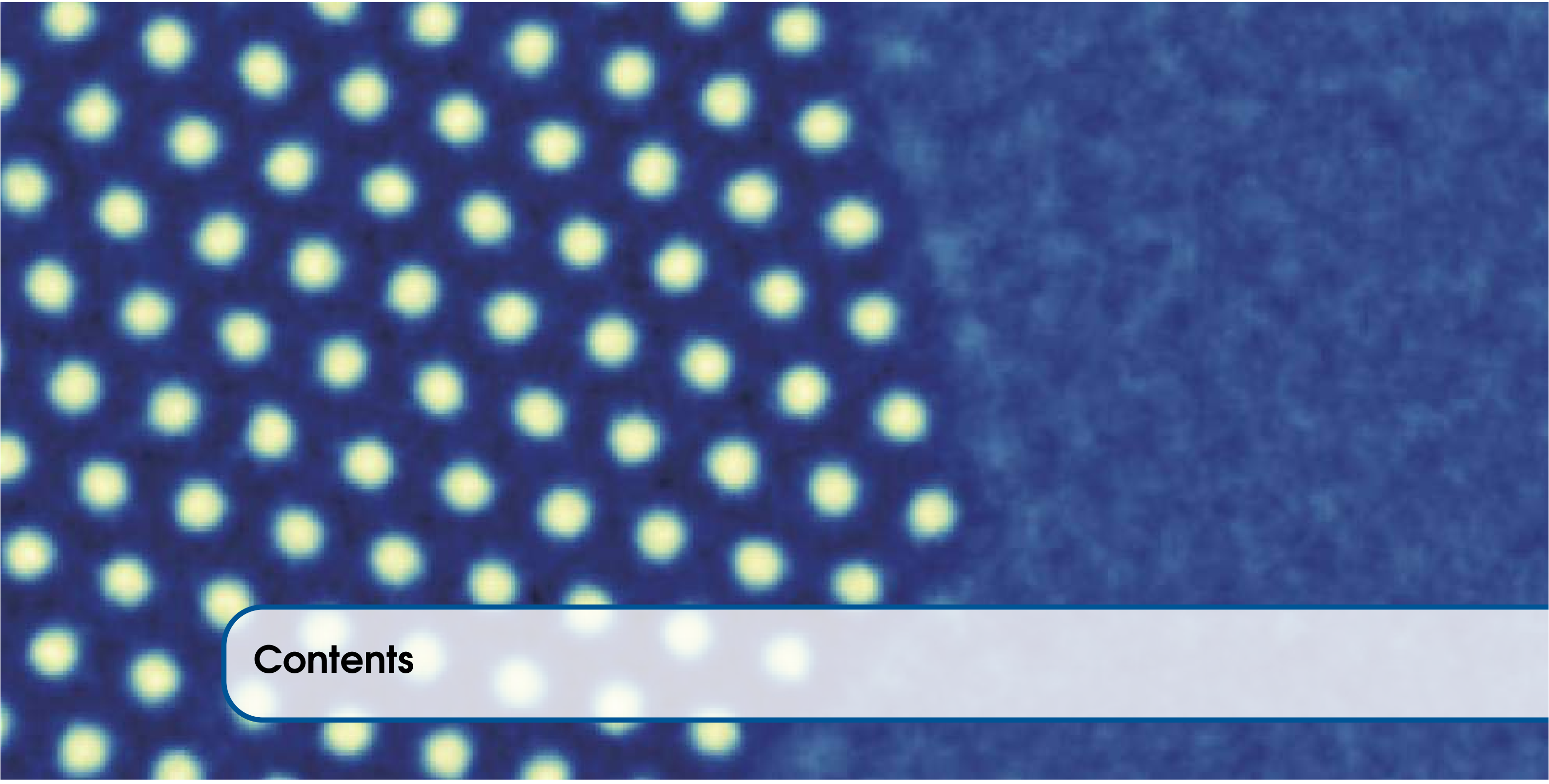
On the cover: Resonant soft X-ray scattering aided by molecular simulation reveals the 3D details of block copolymer assembly [Khaira, G. S.; Doxastakis, M.; Bowen, A.; Ren, J.; Suh, H. S.; Segal-Peretz, T.; Chen, X; Zhou, C; Ferrier, N. J.; Vishwanath, V.; **Sunday**, D. F.; Gronheid, R.; **Kline**, R. J.; **de Pablo**, J.J.; **Nealey**, P.F.]

Editor
Emine Begum Gulsoy, Ph.D.
CHiMaD Associate Director

CHiMaD Headquarters
Northwestern University, O.T. Hogan Biological Sciences Building, Suite 1160
2205 Tech Drive, Evanston, IL, USA 60208
Ph: (847)467-6247 chimad.northwestern.edu | chimad@northwestern.edu

This work was performed under the following financial assistance award 70NANB14H012 from U.S. Department of Commerce, National Institute of Standards and Technology as part of the Center for Hierarchical Materials Design (CHiMaD).

CHiMaD 2016



Contents

I Center for Hierarchical Materials Design

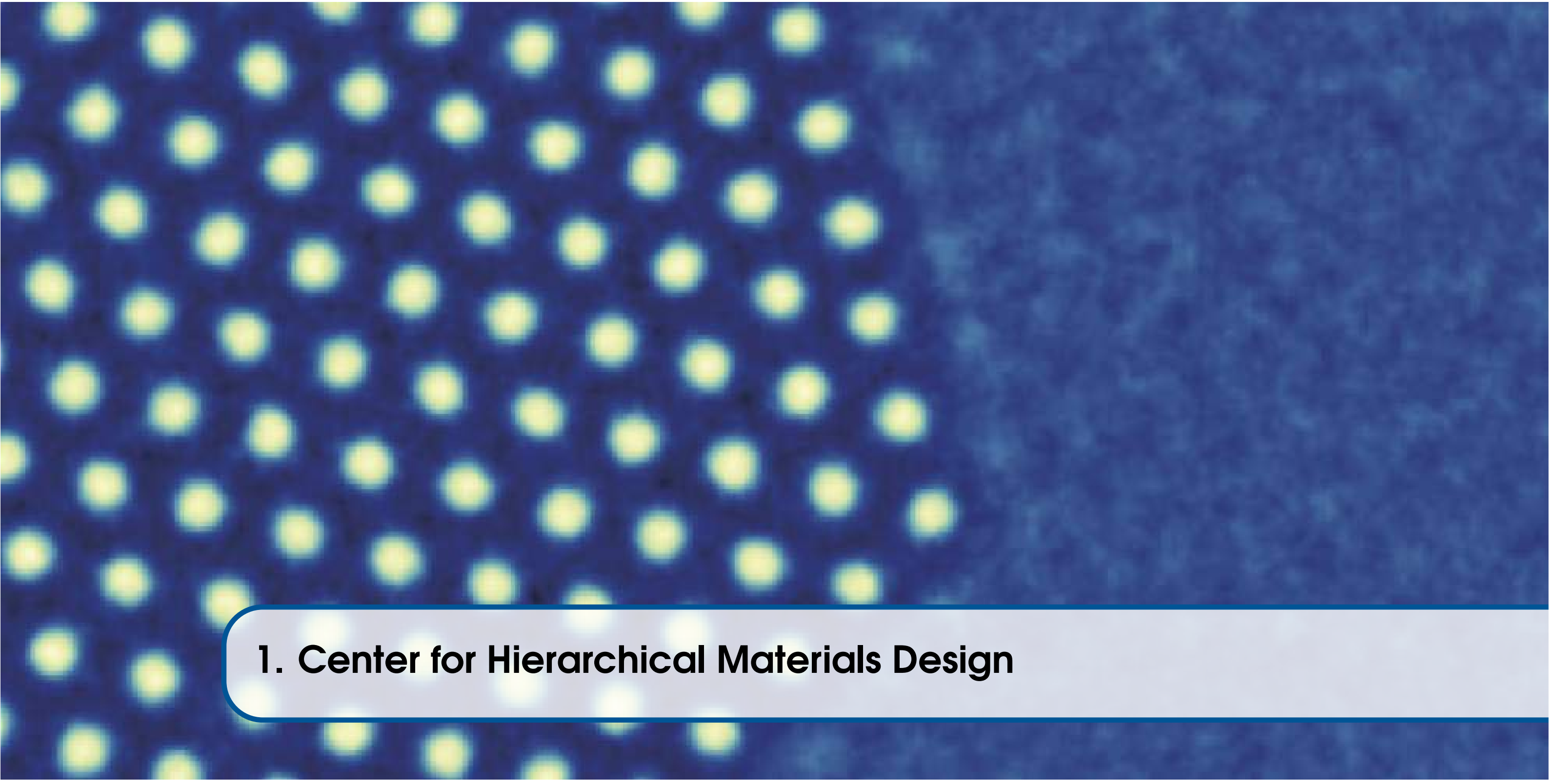
II CHiMaD Research

III CHiMaD Seed Groups

IV CHiMaD Tools & Facilities

V Outreach

Center for Hierarchical Materials Design



1. Center for Hierarchical Materials Design

Foreword

We are pleased to present the third annual report of the Center for Hierarchical Materials Design (CHiMaD), the National Institute for Standards and Technology (NIST) Center of Excellence in Advanced Materials. CHiMaD has become a focal point, both nationally and internationally, for the Materials Genome Initiative (MGI). We are committed to achieving the goals of the MGI through the development of broad research and outreach programs that involve participants from universities, national laboratories and companies. Bringing together researchers with expertise in computation, data science, and experiment to focus on the design of new materials is at the core of both the MGI and the CHiMaD. These collaborative efforts illustrate the power of incorporating experimental and computational databases in the materials design process.

Along with scientists and engineers from the National Institute for Standards and Technology, we are demonstrating the impact and potential of the MGI by designing novel materials ranging from cobalt superalloys and 2D heterostructures for electronics to polymer matrix composites. The CHiMaD involves 39 principal investigators, 52 NIST scientists and engineers, 26 postdoctoral research fellows, 63 graduate students and 5 undergraduate students working in the CHiMaD use-case groups. This report presents the objectives and accomplishments of our use-case groups, seed groups, and multiple tool development efforts. The breadth of our portfolio allows us to interact with a diverse array of industrial collaborators such as Owens Corning, Intermolecular and Northrop Grumman. We are also a resource for the Nation through the sponsorship of workshops, on topics ranging from Phase Field Methods to Impact Mitigating Materials for Body Protection and Materials Data and Analytics for Materials Research, as well as by providing databases for the community such as Nanomine, χ-DB and data repositories such as the Materials Data Facility (MDF). This year, the reach of the MDF has been expanded through our recent NSF award to be the materials-focused spoke on integrated materials design for the Midwest Big Data Hub as part of the national Big Data Innovation program. This effort also brings together CHiMaD, University of Michigan, University of Illinois at Urbana-Champaign, and University of Wisconsin. An outgrowth of the Phase Field Methods workshops has been the establishment of community based benchmark problems for phase field codes; the paper describing the problems was recognized as an editor's choice. We are impacting materials design education throughout the country. For example, all the winners of the ASM undergraduate materials design competition for the past two years are ASM-CHiMaD materials design toolkit awardees, along with Northwestern University. In addition to these community building efforts, our materials design work continues to impact the community through the publication of high impact papers, technology transfer to industry, and high-profile talks.

Our national and international visibility and many design efforts are moving forward with great speed. We are making the promise of the Materials Genome Initiative a reality. We look forward to another exciting year.

Peter Voorhees, Juan de Pablo, Gregory Olson
CHiMaD Co-Directors

Mission and Vision

> *Accelerating materials discovery and commercialization by design and development of hierarchical methods and materials and enabling the complete integration of computation, experimentation and databases by building a strong community of current and future researchers*

Center for Hierarchical Materials Design (CHiMaD) is a NIST-sponsored center of excellence for advanced materials research that is focused on developing the next generation of computational tools, databases and experimental techniques in order to enable the accelerated design of novel materials and their integration to industry, one of the primary goals of the *Materials Genome Initiative (MGI).*

This Chicago-based consortium includes Northwestern University (NU) as the lead, University of Chicago (UChicago), Northwestern-Argonne Institute for Science and Engineering (NAISE), a partnership between Northwestern University and Argonne National Laboratory (ANL), and the Computational Institute (CI), a partnership between University of Chicago and Argonne National Laboratory. The consortium is also partnered with Questek Innovations (QT), a pioneering materials design company, ASM International and Fayetteville State University.

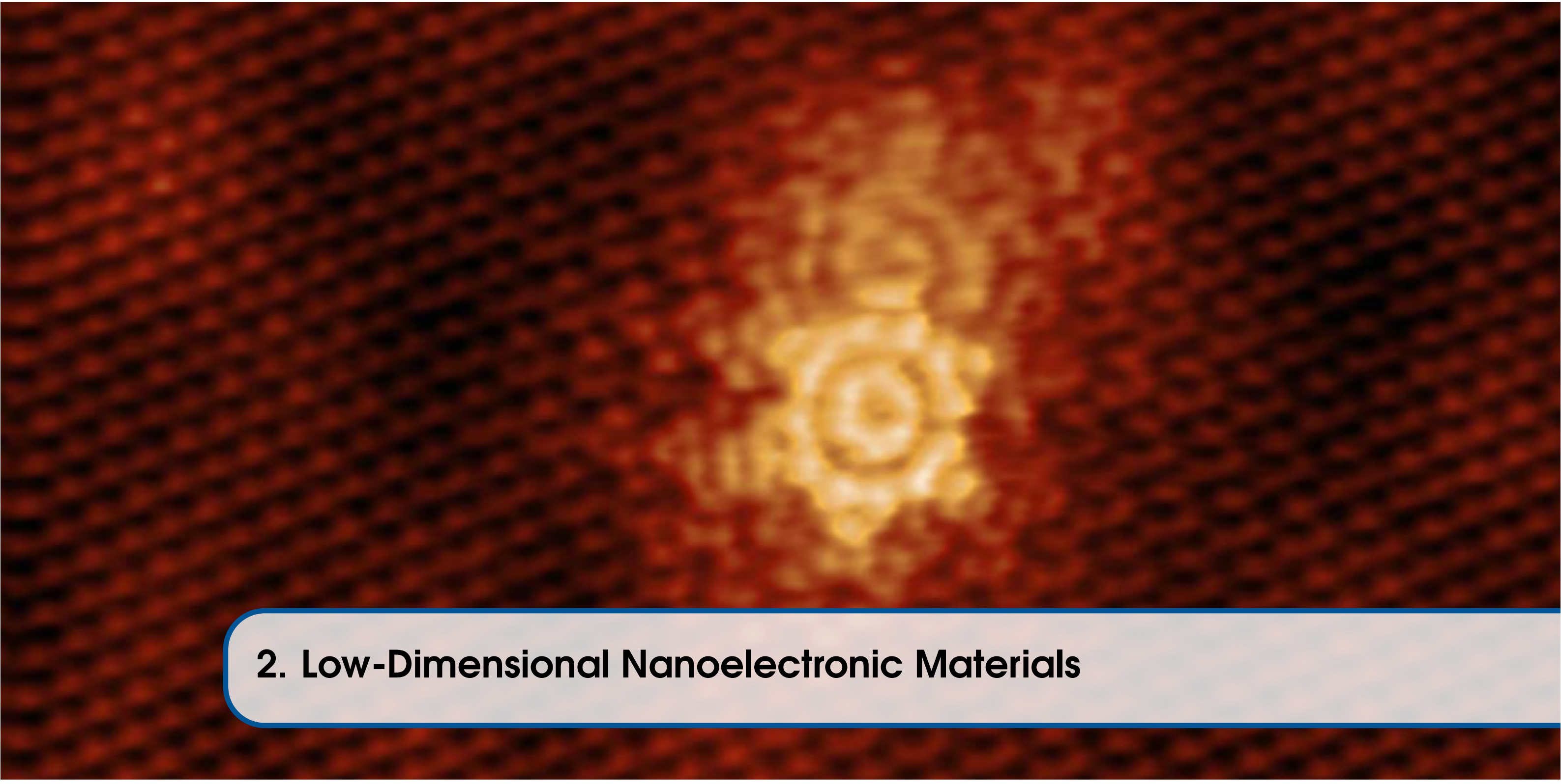
Designing novel materials of specific properties for a particular application requires simultaneously utilizing physical theory, advanced computational methods and models, materials properties databases and complex calculations. This approach stands in contrast to the traditional trial-and-error method of materials discovery. CHiMaD aims to focus this approach on the creation of novel *hierarchical materials* which exploit distinct structural details at various scales, from the atomic on up, to obtain enhanced properties. The center's research focuses on both organic and inorganic advanced materials in fields as diverse as self-assembled biomaterials, smart materials for self-assembled circuit designs, organic photovoltaic materials, advanced ceramics and metal alloys.

Objectives

- To *foster* hierarchical materials discovery, in accordance with the goals of MGI and NIST, by developing the next generation of computational tools, databases and experimental techniques.
- To *connect* and *convene* the current experts and the next generation of scientists by advancing the multi-disciplinary and multisector communication through workshops, seminars, training opportunities and meetings
- To *provide* opportunities to transition new breakthroughs in advanced materials to industry
- To *adopt* a seamless integration of prediction, measurement and interpretation
- To *maintain* and *advance* the collective knowledge on material systems and methodologies and to *serve*, together with NIST, as a national resource for verified codes and curated databases that will enable proliferation of a materials-by-design strategy and materials discovery through US industry partners
- To *build* on the established success in metal alloy systems to prove generality of the materials-by-design approach through application to both inorganic and organic advanced systems for both structural and multifunctional applications
- To *expand* the 3D and 4D characterization methods for hard materials design and to bring such methods to the forefront of soft materials design

II

CHiMaD Research



2. Low-Dimensional Nanoelectronic Materials

Mark Hersam (NU), Lincoln Lauhon (NU)

Albert Davydov (NIST), Francesca Tavazza (NIST), Benjamin Burton (NIST), Arunima Singh (NIST), Sergiy Krylyuk (NIST), Deepak Sharma (NIST)

Significance

The Low-Dimensional Nanoelectronic Materials use-case group seeks to understand and realize p-type and n-type doping in the low-dimensional limit. Since low-dimensional nanoelectronic materials have exceptionally high surface area to volume ratios, doping can be realized via two qualitatively different pathways: conventional substitutional doping and surface chemical functionalization. Furthermore, contacts can be designed to selectively inject carriers into the conduction or valence band, thus providing effective n-type and p-type behavior, respectively. Experimental methods in this use-case group include charge transport measurements, optical spectroscopy (e.g., absorbance, photoluminescence, and Raman spectroscopy), and high-resolution microscopy (e.g., scanning probe microscopy, electron microscopy, and atom probe tomography). These experimental methods are complemented by an extensive suite of computational techniques including multi-scale modeling, molecular dynamics, density functional theory, and finite element methods. The interplay between experiment and computation accelerates the understanding and design of doped low-dimensional nanoelectronic materials and their heterostructures.

2.1 Design Goals

The Low-Dimensional Nanoelectronic Materials Use-Case Group is pursuing the following design goals:

Substitutional Doping of Low-Dimensional Semiconductors. Substitutional doping is the most common means of controlling carrier concentration in bulk semiconductors. In the low-dimensional limit, substitutional doping is expected to play the same role, although the reduced degrees of freedom for charge transport suggest that this doping strategy will have greater deleterious effects on charge carrier mobility than in bulk materials. By combining unique characterization methods (e.g., atom probe tomography) with advanced computational methods (e.g., density functional theory), the design trade-offs between carrier concentration and mobility can be quantitatively understood and exploited to optimize materials properties for low-dimensional nanoelectronic devices.

Surface Chemical Functionalization Doping of Low-Dimensional Semiconductors. Since low-dimensional semiconductors have exceptionally high surface area to volume ratios, carrier concentration can also be controlled via surface chemical functionalization doping. The vast phase space for candidate surface chemical treatments necessitates an MGI-based approach to this design problem. Specifically, electron withdrawing and electron donating chemistries are being screened experimentally and computationally to realize controlled p-type and n-type doping, respectively. The results of this work are informing ongoing efforts to optimize spatially varying doping profiles that serve as the basis of many nanoelectronic devices including p-n junction diodes and transistors.

Developing Heterojunctions Consisting of Low-Dimensional Semiconductors. Since low-dimensional semiconductors have self-passivating surfaces, they can be directly integrated into van der Waals heterostructures without the epitaxial constraints of bulk semiconductors. Since this attribute implies a much greater number of heterojunction possibilities compared to bulk materials, efficient experimental and computational screening methods are required. Specific design goals include engineering of the band alignment and charge/energy transfer across heterojunction interfaces, which will allow optimization of nanoelectronic device metrics such as anti-ambipolarity, operating frequency, and optoelectronic response.

2.2 Significant Accomplishments in 2016

Few-layer black phosphorus (BP) is a two-dimensional semiconducting material with high carrier mobilities (up to 1000 $cm^2/V-s$) and anisotropic properties that are promising for next-generation nanoelectronics. However, the chemical reactivity of few-layer BP has limited its applicability due to rapid degradation over a few hours in ambient conditions. In addition, reliable doping methods for BP have been elusive. To overcome these limitations, **Hersam** (NU) has utilized the chemical reactivity of BP to covalently functionalize the surface of mechanically exfoliated few-layer BP with 4-nitrobenzene diazonium and 4-methoxybenzene diazonium tetrafluoroborate salts (Figure 2.1). This chemical modification results in a controllable p-type doping of the BP that significantly improves BP field-effect transistor (FET) device metrics. In addition to higher hole carrier mobility, FETs fabricated from the diazonium-doped few-layer BP exhibit an increase in current on/off ratio by more than 100-fold. Furthermore, the diazonium functionalization passivates the few-layer BP surface, preventing degradation for over 10 days of ambient exposure. Overall, this work realizes a surface chemical functionalization approach that simultaneously controls doping and imparts chemical passivation to BP, thereby enhancing its applicability to nanoelectronic technologies. The results of this study were recently published in *Nature Chemistry* [25.13].

2.3 Research Accomplishments

Atom Probe Tomography of Two-Dimensional Materials. **Lauhon** performed the first 3D compositional analysis of a 2D layered compound, Ag doped $(PbSe)_5(Bi_2Se_3)_3$, by combined atom probe tomography (APT) analysis and density functional theory (DFT)

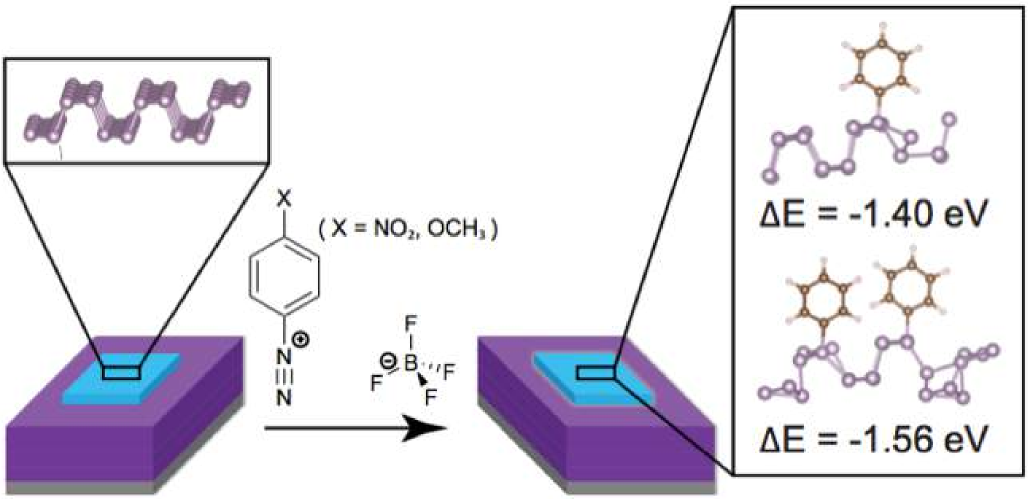


Figure 2.1: Depiction of the reaction scheme of benzene-diazonium tetrafluoroborate derivatives with 2D black phosphorus (blue) on a SiO_2 (purple) on Si (gray) substrate. The calculated lattice distortions resulting from adsorption of the aryl groups, and their respective adsorption energies, are shown on the right.

calculations. Prior work had shown that APT can resolve alternating $PbSe$ and Bi_2Se_3 layers. Additional analysis revealed correlations in the distribution of Ag atoms that are in agreement with new DFT results on larger unit cell sizes (Figure 2.2a). The experimental $Ag-Ag$ radial distribution function (RDF) shows an increased probability of finding Ag atoms ~7Å apart (Figure 2.2b), indicating a pairwise correlation in Ag dopant distribution. With RDF analyses within each sublayer and between sublayers, this $Ag-Ag$ pairing was proven to occur primarily between Ag atoms in adjacent Bi_2Se_3 and $PbSe$ sublayers. The activity of the dopant and its effect on electronic properties depend strongly on its local configuration. Hence, these results provide a methodological foundation for controlled doping of 2D materials. Based on these results, **Lauhon** (NU) and **Davydov** (NIST) published the following paper in *Nano Letters* [25.12].

In an effort to extend APT analysis to other classes of 2D materials, new sample preparation methods were developed for transition metal dichalcogenides (TMDCs), which are significantly more challenging to analyze by APT than conventional semiconducting materials. Accordingly, a structure was designed to prevent fractures caused by weak interlayer bonding in TMDCs. Specifically, a thin layer of metal was deposited onto a Si substrate, and then few-layer TMDC flakes were exfoliated and transferred onto the thin film, followed by the deposition of the same metal. A focused ion beam (FIB) "liftout" procedure was performed to extract a wedge containing TMDC flakes and to mount the wedge onto Si posts after rotating 90 degrees. Mounted wedge fragments were sharpened until only metal and TMDC remained (Figure 2.2c). Preliminary results of APT analysis of SnS grown by atomic layer deposition were obtained, and few-layer SnS was observed in the reconstruction (Figure 2.2c). Ongoing research is focusing on analyzing dopants and impurities in SnS in addition to extending this method to other 2D materials.

Defects in Rotationally Commensurate MoS_2 *on Epitaxial Graphene.* Due to their potential for application in electronic and optoelectronic devices, atomically thin transitional metal dichalcogenide/graphene heterostructures are of high interest for next-generation nanoelec-

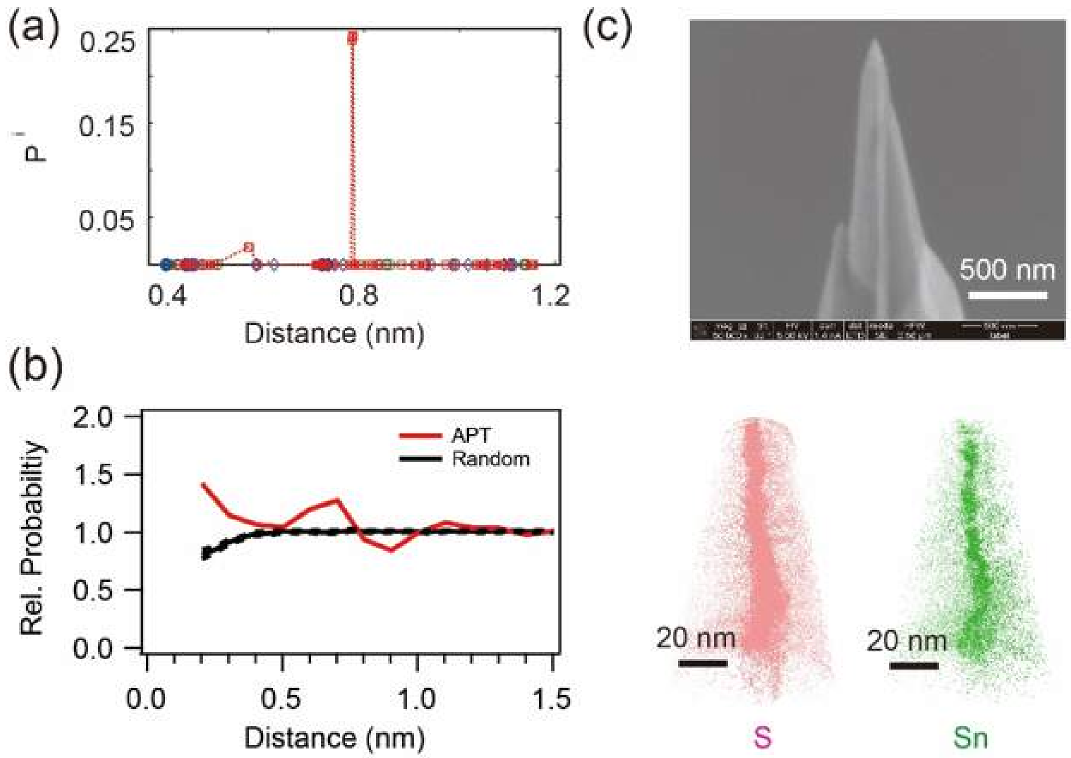


Figure 2.2: (a) Probabilities of the occurrence of $Ag-Ag$ configurations at $300K$ from DFT calculations. (b) $Ag-Ag$ radial distribution function from APT reconstruction compared with that of Ag atoms randomly substituted for Bi and Pb atoms. (c) SEM image of a sharpened tip from a $Ag-SnS-Ag$ sandwich structure and the distribution of S and Sn in the APT reconstruction.

tronics. The recent realization of rotationally commensurate MoS_2 on epitaxial graphene (EG) by **Hersam** (NU) has provided an ideal platform for the study of two-dimensional heterojunctions. Using ultra-high vacuum scanning tunneling microscopy, **Hersam** (NU) has investigated the intrinsic structural defects of rotationally commensurate MoS_2 on EG, namely, point defects and grain boundaries. As a result of the van der Waals epitaxy between MoS_2 and EG, the point defect density was found to be lower than MoS_2 grown on other substrates. The electronic consequences of the MoS_2 grain boundaries were also characterized and found to result in MoS_2 band gap reductions of $\sim 0.8eV$ and $\sim 0.5eV$ for 30° and 60° grain boundaries, respectively. This work has been published in *Journal of Physical Chemistry C* [25.11]

Direct Growth of Monolayer MoS_2 on Ultrathin Al_2O_3 Dielectrics. One of the most promising applications for two-dimensional transition metal dichalcogenides is low-power electronics. The integration of MoS_2 with high-κ dielectrics, such as Al_2O_3 grown by atomic layer deposition (ALD), is necessary to achieve devices with low operating voltages. However, doping control in the fabrication of scalable monolayer MoS_2/high-κ dielectric heterostructures has been insufficient to achieve the enhancement-mode devices necessary for low-power operation. To address this problem, in an inter-use-case group collaboration with **Bedzyk** (NU) and **Marks** (NU), **Hersam** (NU) has demonstrated direct chemical vapor deposition (CVD) growth of monolayer MoS_2 on $20nm$ thick ALD Al_2O_3. This method overcomes the doping issues associated with previous methods of MoS_2 integration with high-κ dielectrics including: (a) unpredictable doping from the inhomogeneous residues introduced during transfer of MoS_2 onto high-κ dielectrics; (b) large n-type doping that occurs following deposition of high-κ dielectrics on top of MoS_2. In contrast, directly-grown CVD MoS_2 shows superior performance in low-power device figures of merit and supports the prospect of scalable MoS_2/high-κ dielectric heterostructures as a pathway to low-power nanoelectronics.

Publishing Nanoelectronic Material Datasets in the Materials Data Facility. As an early adopter and contributor to the Materials Data Facility (MDF), **Hersam** (NU) and **Lauhon** (NU) in collaboration with **Davydov** (NIST), **Singh** (NIST), and **Tavazza** (NIST) have published several low-dimensional nanoelectronic material datasets based on CHiMaD-supported publications and earlier work that is of relevance to ongoing and future CHiMaD efforts. Currently, the datasets make use of the flexible access control feature of the MDF, requiring permission for full-access. Three of the six datasets uploaded correspond to the raw data linked to CHiMaD publications [25.10, 25.11, 25.12] and are comprised of results from a variety of experimental techniques. Please see section 10.9 for the complete list of contributed data.

2.4 Collaborations

2.4.1 CHiMaD Collaborations

Doping of Black Phosphorus via Chemical Functionalization
*Tobin **Marks** (NU), Mark **Hersam** (NU)*
Few-layer black phosphorus was functionalized using diazonium chemistry to achieve controllable p-type doping for improved transistor metrics and passivation against ambient degradation. This work resulted in the following collaborative publication [25.13].

Direct Growth of Monolayer MoS_2 on Ultrathin Al_2O_3 Dielectrics
*Michael **Bedzyk** (NU), Tobin **Marks** (NU), Mark **Hersam** (NU)*
Monolayer MoS_2 was directly grown by chemical vapor deposition on $20nm$ thick Al_2O_3 grown by atomic layer deposition. The doping control enabled by this transfer-free method of MoS_2/high-κ dielectric heterostructure fabrication resulted in enhancement-mode devices for low power electronics. This collaborative work has been accepted for publication in *Applied Physics Letters*.

Sample preparation for APT analysis of few-layer 2D materials
*Mark **Hersam** (NU), Lincoln **Lauhon** (NU)*
Lauhon (NU) group used the **Hersam** (NU) group expertise in sample preparation of few-layer 2D materials for atom probe tomography.

2.4.2 NIST Collaborations

Temperature-Driven Phase Transition in $MoTe_2$
*Albert **Davydov** (NIST), Mark **Hersam** (NU)*
Davydov (NIST) achieved a reversible phase transition between the 2H and 1T' phases of $MoTe_2$ grown using chemical vapor transport via high temperature annealing. **Hersam** (NU) performed charge transport measurements to confirm 2H and 1T' semiconducting and metallic behavior, respectively. A collaborative manuscript is under preparation on this work.

Charge Transport in Transition Metal Dichalcogenide (TMDC) Alloys
*Albert **Davydov** (NIST), Mark **Hersam** (NU)*

Davydov is growing and supplying bulk crystals of TMDC alloys that are being incorporated into transistor devices by **Hersam** (NU) for charge transport measurements.

Atom Probe Tomography Characterization of Ag doping in $(PbSe)_5(Bi_2Se_3)_{3m}$

*Mercouri Kanatzidis (Northwestern University), Francesca **Tavazza** (NIST), Arunima **Singh** (NIST), Lincoln **Lauhon** (NU)*

Kanatzidis group provided samples of Ag doped $(PbSe)_5(Bi_2Se_3)_{3m}$; **Lauhon** (NU) group characterized Ag doped $(PbSe)_5(Bi_2Se_3)_{3m}$ using atom probe tomography; **Tavazza** (NIST) and **Singh** (NIST) performed DFT calculations at NIST. This work was published in *Nano Letters* [25.12].

S incorporation in $MoTe_2$

*Albert **Davydov** (NIST), Sergiy **Krylyuk** (NIST), Lincoln **Lauhon** (NU)*

Xiaochen Ren, graduate student in **Lauhon** Group, spent extended research time at NIST to collaborate with **Davydov** (NIST) and **Krylyuk** (NIST) to study S incorporation in $MoTe_2$ by annealing $MoTe_2$ in S vapor. $MoTe_2$ crystals were obtained by chemical vapor transport growth. Then $MoTe_2$ crystals and S powders were sealed in the same ampoule and were annealed at 750°C. S was expected to be incorporated into $MoTe_2$ crystals to form $MoTe_{2-x}S_x$, which can be used to tune the bandgap of $MoTe_2$ and improve the superconductivity of 1T' $MoTe_2$. Electrical characterization will be performed by **Lauhon** (NU) group at Northwestern in 2017.

2.4.3 External Collaborations

Doping of Black Phosphorus via Chemical Functionalization

*George Schatz (Northwestern University), Mark **Hersam** (NU)*

Few-layer black phosphorus was functionalized using diazonium chemistry to achieve controllable p-type doping for improved transistor metrics and passivation against ambient degradation. This work resulted in the following collaborative publication [25.13].

Charge Transfer in MoS2-pentacene p-n Heterojunctions

*Emily Weiss (Northwestern University), Mark **Hersam** (NU)*

The charge transfer in a p-n heterojunctions consisting of n-type chemical vapor deposition MoS_2 and an organic adlayer of p-type pentacene are being investigated via transient absorption spectroscopy. This work is likely to lead to a publication in CHiMaD's Year 4.

Solution-Processed Nanoelectronic Materials

*Shashi Jasty (Sigma-Aldrich), Jia Choi (Sigma-Aldrich), Adam Raw (Sigma-Aldrich), Mark **Hersam** (NU)*

A series of solution-processed, printable graphene inks have been formulated by **Hersam** (NU), and are being distributed commercially by *Sigma-Aldrich*. In particular, three products are now available on the *Sigma-Aldrich* website including: (1) Inkjet printable graphene; (2) Gravure printable graphene; (3) Screen printable graphene.

Atom Probe Tomography Characterization of Ag doping in $(PbSe)_5(Bi_2Se_3)_{3m}$

*Mercouri Kanatzidis (Northwestern University), Francesca **Tavazza** (NIST), Arunima **Singh** (NIST), Lincoln **Lauhon** (NU)*

Kanatzidis group provided samples of Ag doped $(PbSe)_5(Bi_2Se_3)_{3m}$; **Lauhon** (NU) group characterized Ag doped $(PbSe)_5(Bi_2Se_3)_{3m}$ using atom probe tomography; **Tavazza** (NIST) and **Singh** (NIST) performed DFT calculations at NIST. This work was published in *Nano Letters* [25.12].

2.5 Technology Transfer

Invention

System and method for anti-ambipolar heterojunctions from solution-processed semiconductors

D. M. Jariwala, V. K. Sangwan, W. Xu, H. Kim, T. J. Marks, M. C. Hersam
U.S. Provisional Patent application published on 7/14/16
Patent Number: US 20016/0204773

This invention describes a method for forming large-area, anti-ambipolar p-n heterojunctions using solution-processed p-type semiconducting single-walled carbon nanotubes (s-SWCNTs) and n-type amorphous indium gallium zinc oxide (a-IGZO) thin films via photolithographic and etching techniques.

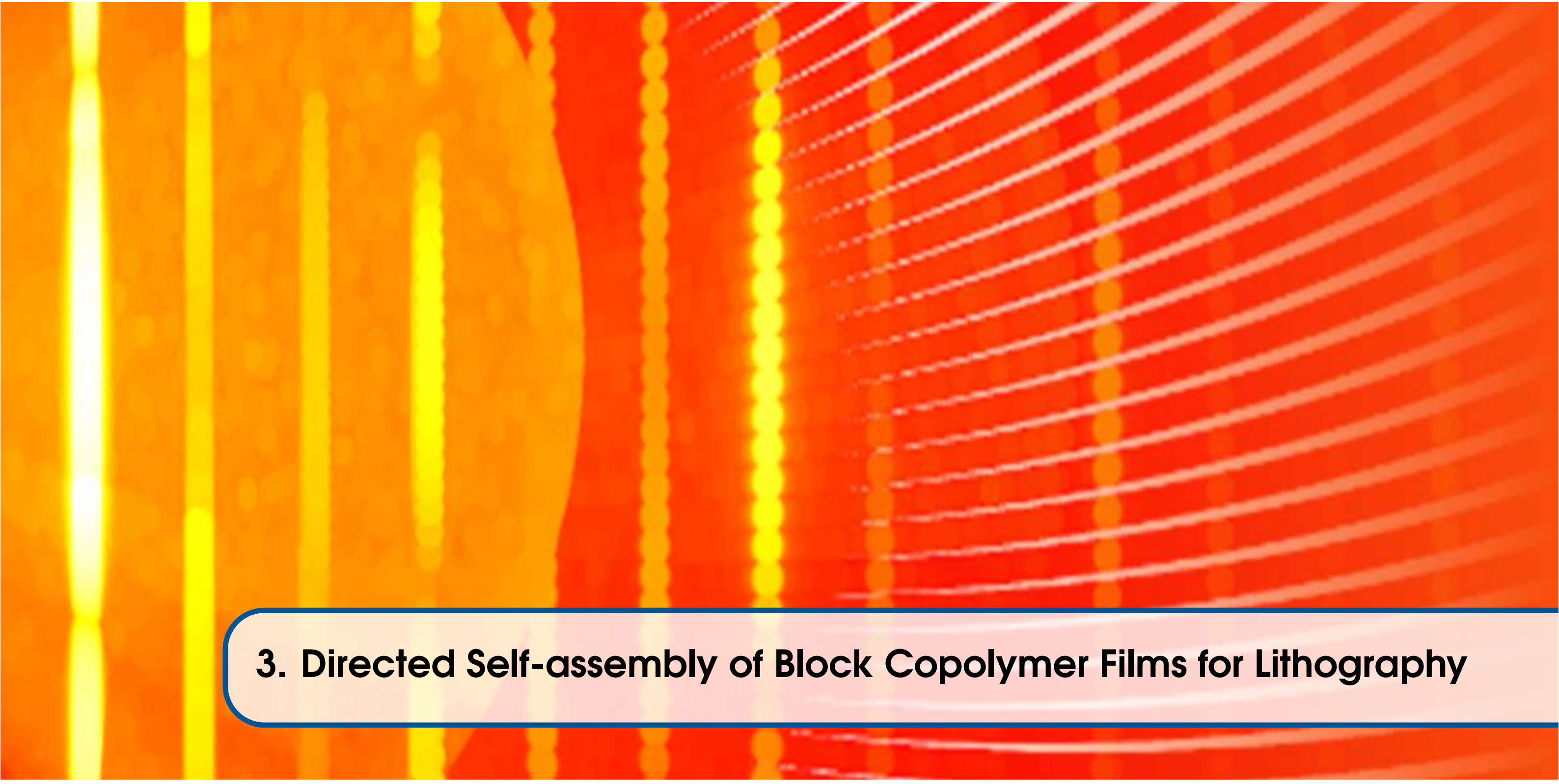
2.6 Publications and Presentations

4 Number of CHiMaD-supported publications in 2016 by Low-Dimensional Nanoelectronic Materials use-case group. Please see chapter 25 for details. [25.10,25.11, 25.12, 25.13]

32 Number of presentations on CHiMaD-supported research given in 2016 by Low-Dimensional Nanoelectronic Materials use-case group members, please see section 24.1 for the complete list.

2.7 CHiMaD Team

Low-Dimensional Nanoelectronic Materials Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Mark Hersam	Principal Investigator	NU/MSE	
Lincoln Lauhon	Principal Investigator	NU/MSE	
Hadallia Bergeron	Graduate Student	NU/MSE	Low-dimensional semiconductor heterojunctions *(Hersam)*
Megan Beck	Graduate Student	NU/MSE	Low-dimensional semiconductor heterojunctions *(Hersam, NSF Fellowship)*
Itamar Balla	Graduate Student	NU/MSE	Low-dimensional semiconductor heterojunctions *(Hersam)*
Xiaochen Ren	Graduate Student	NU/MSE	Substitutional doping and alloy formation in transition metal dichalcogenides *(Lauhon)*



3. Directed Self-assembly of Block Copolymer Films for Lithography

Paul Nealey (UC), Juan de Pablo (UC), Steven Sibener (UC), Heinrich Jaeger (UC), Ian Foster (UC/ANL)

Joseph Kline (NIST), Daniel Sunday (NIST), Debra Audus (NIST), Kenneth Kroenlein (NIST), Adam Hannon (NIST), Jonathan Winterstein (NIST), Alexander Liddel (NIST)

Significance

Directed self-assembly (DSA) of block copolymers (BCPs) has the potential to revolutionize nanomanufacturing. BCPs self-assemble to form densely packed features with highly uniform dimensions and shapes in ordered arrays at the scale of 3 to 50 nm. Chemical pre-patterns or templates may be defined using traditional lithographic materials and processes such as 193 immersion lithography at the scale of 80 nm. By directing the assembly of block copolymer films on the templates, the overall resolution of the lithographic process may be increased by three to four-fold or more and still meet the stringent requirements of manufacturing, including perfection, dimension control, and pattern placement accuracy. The interest and exponential growth in research activity and expenditure is driven in the semiconductor industry by the prospect of manufacturing future generations of computer chips according to Moore's law, without having to invest billions in new fabrication facilities (i.e. based on extreme ultra violet lithography) that may or may not be able to meet the resolution requirements already being demonstrated by DSA. For hard drives, block copolymer lithography is the only known technology to fabricate nanoimprint masters to manufacture bit patterned media at the required storage densities greater than 2 Tera dots/inch^2. This use-case collaborates with Intel, IBM, TOK, Seagate, IMEC and Mentor Graphics.

3.1 Design Goals

Directed Self-assembly of Block Copolymer Films for Lithography use-case group seeks to design block copolymer materials and assembly processes to enable manufacturing via DSA at length scales of 10 nm, scaling to 5 nm, and meet manufacturing constraints with respect to defects ($0.01/\text{cm}^2$), and line edge and width roughness (<1 nm). The structure of the assembled BCP depends on many variables describing material properties (molecular weight, block architecture, interaction parameter χ) and process parameters (temperature, solvent, assembly time, template chemistry and topography, interfacial energies, and surface energies); our design objectives can only be met by developing and validating predicative multi-scale models. Moreover, the immense parameter space requires evolutionary approaches to simultaneously understand and optimize numerous variables, in the context of analysis of experimental data and in the design of new materials and processes. To accomplish our design goals with respect to structure, our priority and main activity is to advance three-dimensional metrology tools and methods, and develop expertise in quantitatively comparing predictive models and experimental data. The focus of former mentioned activities are the independent variables (design criteria)- material properties, template properties, and processing parameters. Molecular simulation-based data analysis is the foundation for delineating complex structure-property-processing relationships and is accomplished by close collaboration with **Kline** (NIST) and **Sunday** (NIST). To accomplish our design goals with respect to design for minimization of defects, we are pioneers in understanding the dominant role of the dynamics and evolution of structure formation. Again, ultra-high information experiments involving high-speed AFM imaging are being analyzed in conjunction with predicative models that include dynamic information, leading to the determination of the key material and process criteria to meet manufacturing constraints.

3.2 Significant Accomplishments in 2016

A key challenge in the advancement of DSA for sub-10 nm semiconductor nanofabrication is the development of quantitative metrology capable of probing hidden three-dimensional structures and offering molecular-level insight. Through extensive partnership with NIST, our use-case group has exploited CDSAXS as a technique to capture the details of the three-dimensional structure of block copolymer domains, fluctuations of domain interface through three-dimensions as well as molecular-level distribution and architecture all as a function of materials, processing and boundary conditions used in DSA. Specifically, we accomplished the following:

- Investigated the 3D structures resulting from different DSA materials including PS-PMMA and PS-P2VP as well as different DSA processes such as template commensurability and topography (**Nealey** (UC), **de Pablo** (UC))
- Developed the experimental techniques as well as the data analysis methodology to characterize DSA structures with Grazing Incidence Small Angle X-ray Scattering, to complement CDSAXS measurements and arrive at a comprehensive description of the structures (**Nealey** (UC), **de Pablo** (UC), **Jaeger** (UC))
- Developed physics based coarse-grain models to analyze experimental data from scattering techniques, directly linking structural information to material properties. This MGI approach to predictive model development and validation is unprecedented in its power to provide optimized independent variables for the design of next generation DSA systems (**Nealey** (UC), **de Pablo** (UC), **Jaeger** (UC))
- Established DSA process with ionic liquid addition to enable PS-PMMA for sub-10 nm fabrication. Used soft X-ray reflectivity to probe the reduction in interfacial width due to ionic liquid addition (**Nealey** (UC))

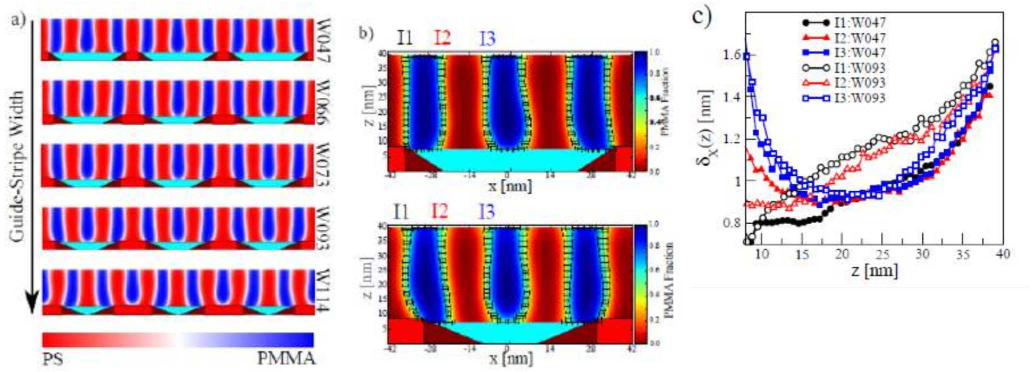


Figure 3.1: 3D Characterization of DSA using CDSAXS. (a) Average cross-sections for samples with different template critical dimensions showing shape variations through the film thickness. (b) Positional fluctuations of the interface with regard to its location on the template. (c) Fluctuation profile in the thickness direction showing increased fluctuations at the top surface.

- Investigated the effect of molecular architecture on the interfacial width of block copolymers using soft X-ray reflectivity, offering insights on DSA material and process design (**Nealey** (UC), **de Pablo** (UC))
- We elucidated the relationship between the kinetic process and defectivity in DSA. Using high-speed AFM, we continuously examined local morphological changes in-situ during thermal annealing and traced the origin and fate of defective structure. Understanding defect kinetics paves the way for better process design and the application of DSA in high-volume manufacturing (**Nealey** (UC), **Sibener** (UC))

3.3 Research Accomplishments

3D characterization of block copolymer DSA using Critical Dimension Small Angle X-ray Scattering. Over the Year Three funding period, the **Nealey** (UC) group continued to build on the extensive and productive collaboration with NIST and the **de Pablo** (UC) group to probe the detailed 3D structures in block copolymer DSA. Leveraging our nanofabrication capabilities as well as our long-time partnership with *IMEC*, we systematically investigated the 3D structures resulting from different DSA materials including PS-PMMA and PS-P2VP as well as different DSA processes such as template commensurability and topography. Utilizing simulation-based data analysis, we were able to delineate the contributions of intrinsic interfacial width and positional fluctuations to the overall blurring of the interface and track the positional fluctuations through three dimensions. Understanding of the 3D structures and interfacial profiles allowed us to address key processing concerns for the implementation of DSA in semiconductor manufacturing and facilitated the path-finding for the development of materials and conditions for future DSA processes, Figure 3.1.

Complementary X-ray characterization using Grazing Incidence Small Angle X-ray Scattering. The concept of combining data from complementary experiments in order to arrive at a comprehensive description of a material has been a long-standing goal in the development of novel materials and processes. To complement CDSAXS analysis, the **Nealey** (UC) and **de Pablo** (UC) groups, in collaboration with **Kline** (NIST) and **Sunday** (NIST) have developed the experimental techniques as well as the data analysis methodology to characterize DSA structures with Grazing Incidence Small Angle X-ray Scattering. Compared to

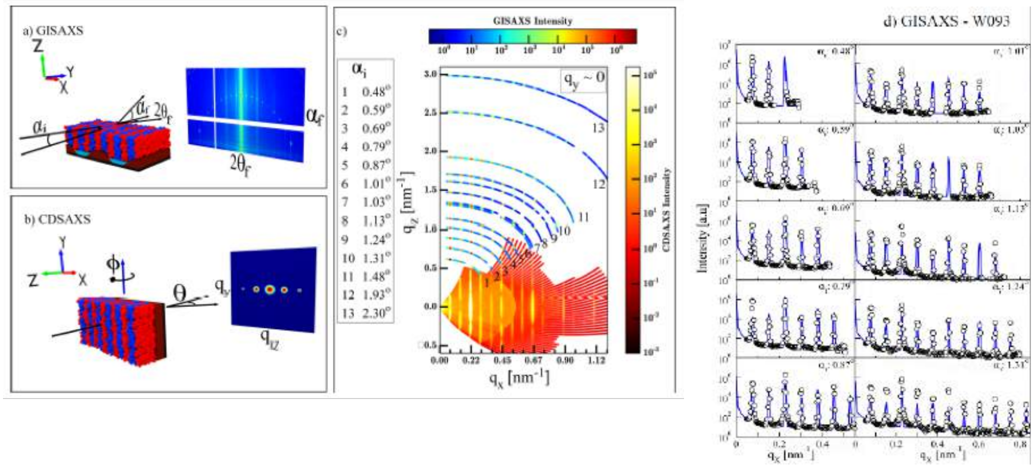


Figure 3.2: (a-b) Schematics of GISAXS and CDSAXS experimental setup. (c) Experimental data from both metrologies showing complementary mapping of the q space. (d) GISAXS scattering profile generated by modeled structure closely fits the experimental data.

CDSAXS, GISAXS probes significantly larger sample area and offers enhanced resolution especially in the thickness direction. Molecular simulation based data analysis helps to reconcile the data from both metrologies and arrive at one detailed description of the sample structure with superior quality than that available from the individual techniques alone, Figure 3.2.

Molecular simulation based X-ray analysis relates structures to thermodynamic properties. Through extensive internal collaboration between the **Nealey** (UC), **de Pablo** (UC) and **Jaeger** (UC) groups, we have developed physics based coarse-grain models to analyze experimental data from scattering techniques capable of probing the complex structures commonly found in the directed self-assembly of block copolymers. The technique not only structurally characterizes the average morphology of a periodic DSA film, but also furnishes fundamental thermodynamic information otherwise unavailable in a manner pertinent to the simulation model, directly linking structural information to material properties. The thermodynamic information extracted by the simulation and metrology can serve to develop tools for predictive modeling and better clarify which of the numerous process conditions must be adjusted to achieve a desirable, defect-free morphology. Such a method can greatly shorten the development cycle and advance our knowledge of these materials to the point where significant progress can be made in applying them to large-scale industrial processes in semiconductor manufacturing, Figure 3.3

Ionic liquid addition for the directed self-assembly of sub-10 nm features. To overcome the resolution limit of traditional *PS-b-PMMA*, ionic liquid (IL) was blended into disordered *PS-b-PMMA* to achieve substantially higher χ than the pure block copolymer. Meanwhile, the change in surface and interfacial properties is still manageable so that the process is compatible with thermal annealing and free of top-coat. Through extensive collaboration with *TOK* Japan and *IMEC* Belgium, the **Nealey** (UC) group accomplished for the first time sub-10 nm DSA of *PS-b-PMMA/IL* blends with half pitch down to 8.5 nm in 300 mm production-level clean room based on the LINE flow which was developed by **Nealey** (UC) group and implemented in *IMEC* years ago. In addition, closely collaborating with **Kline** (NIST) and **Sunday** (NIST), the **Nealey** (UC) group was able to delineate the impact of χ

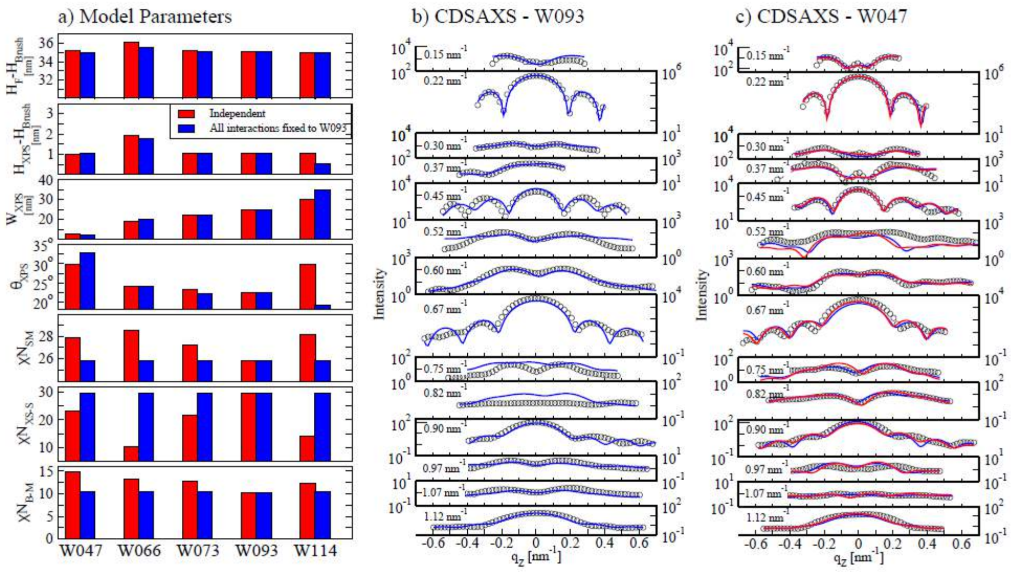


Figure 3.3: Theory and simulation based analysis of X-ray scattering experiments. A single set of material parameters (a) were used to successfully fit the scattering profiles from samples with different template geometries (b) (c). The fine-tuned parameters can then be used for predictive modeling.

on interfacial width and line roughness. With ionic liquid addition, it was revealed by soft x-ray reflectivity that the interfacial width between blocks was significantly narrowed, which well represents more than double increase in χ. To transfer the fundamental understanding towards industrial fabrication end, DSA of *PS-b-PMMA* were compared before and after *IL* addition showing little improvement of line edge roughness after *PMMA* removal, thus indicating that instead of χ increase, other factors like enhanced etch contrast might be more dominant in roughness healing of high-χ materials, Figure 3.4.

Probing interfacial width in PS-P2VP block copolymers using soft X-ray reflectivity. Variations in polymer architecture can work in concert with new monomer chemistries to drive DSA into ever-smaller dimensions and higher resolutions. The interfacial width between two materials is a potential limiting factor in the utility of these new materials. Collaborating with **Kline** (NIST) and **Sunday** (NIST), the **Nealey** (UC) group investigated the interfacial width between *PS* and *P2VP* for different polymer architectures, i.e. AB diblock vs ABA triblock, as well as for diblocks with different molecular weights. Utilizing soft X-ray reflectivity, we demonstrated that both the diblock and triblock with similar periodicities had equivalent interfacial widths. In addition, diblock *PS-P2VP* with higher molecular weights was shown to have a slightly sharper interface. Understanding the influence of molecular architectures on interfacial width would facilitate the design of DSA materials to achieve higher resolution and lower line edge roughness for lithographic applications, Figure 3.5.

In-situ AFM study of the kinetics in directed self-assembly. Theory and simulation have suggested that the DSA defects are thermodynamically unstable and likely represent kinetically trapped states. In close partnership with the **Sibener** (UC) group, the use-case have investigated the kinetics of thermal annealing of *PS-b-PMMA* on chemically patterned substrates using high speed AFM. Video-rate non-destructive imaging uniquely allows us to continuously examine local morphological changes in order to trace the origin and fate

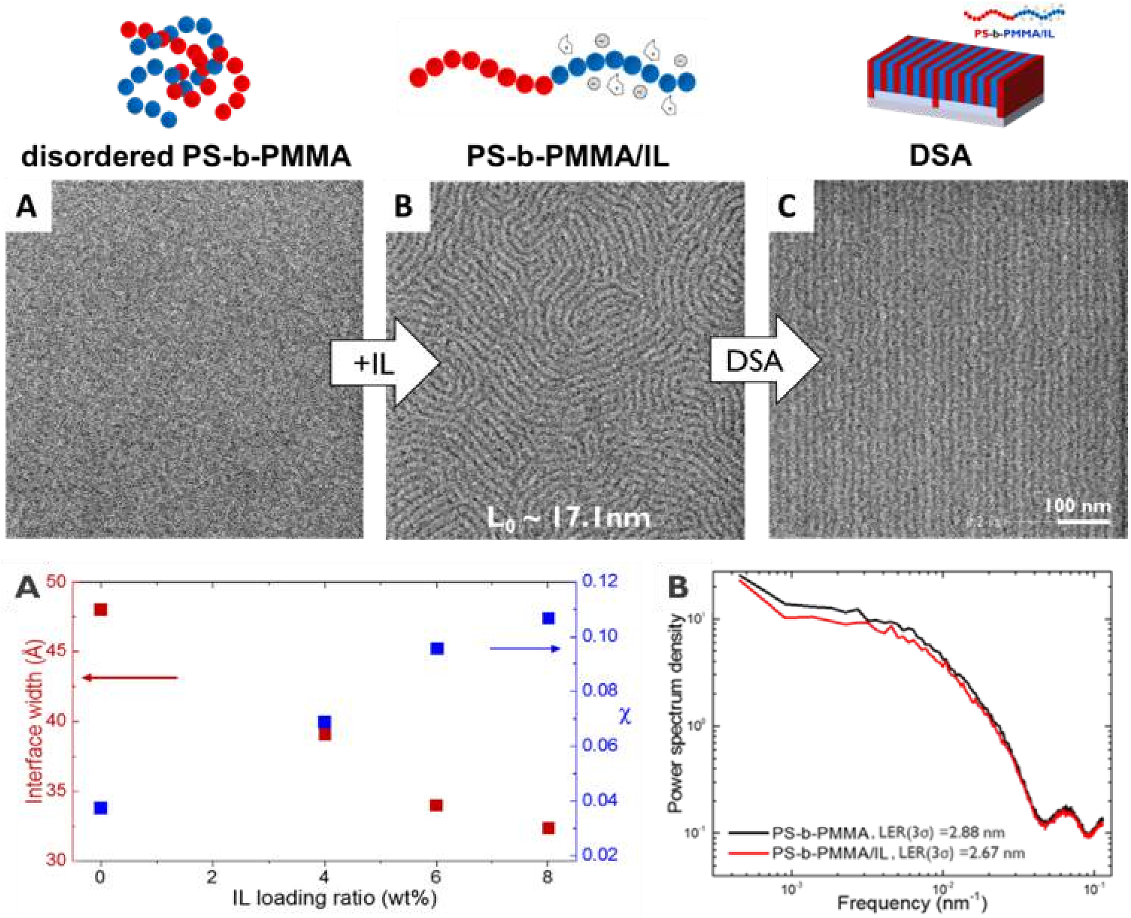
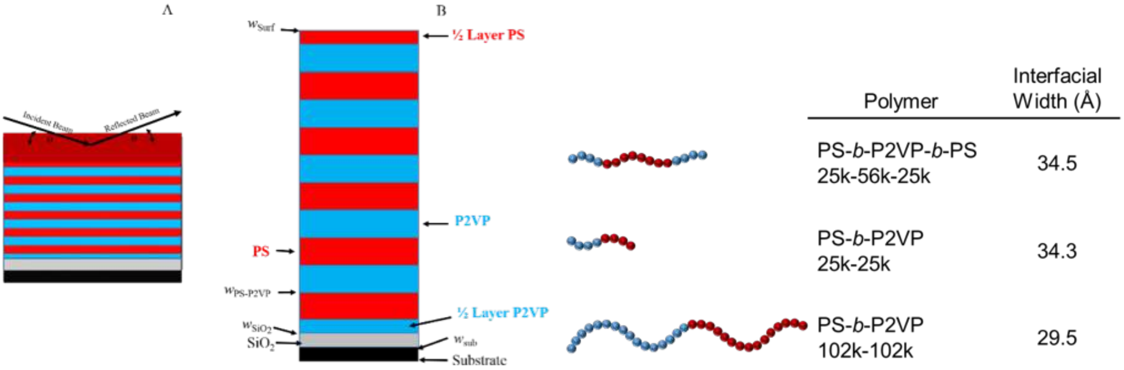


Figure 3.4: Top: (A-C)Addition of ionic liquid facilitates the phase separation of PS-b-PMMA and DSA of 8.5 nm half-pitch lines were demonstrated, Bottom: (A-B) Reflectivity experiments in collaboration with NIST showed that ionic liquid increased the Flory-Huggins parameter between the polymer blocks and reduced the interfacial width.



Polymer	Interfacial Width (Å)
PS-*b*-P2VP-*b*-PS 25k-56k-25k	34.5
PS-*b*-P2VP 25k-25k	34.3
PS-*b*-P2VP 102k-102k	29.5

Figure 3.5: (Left) Soft X-ray reflectivity experimental setup. (Right) Interfacial widths for polymers with different architectures and molecular weights.

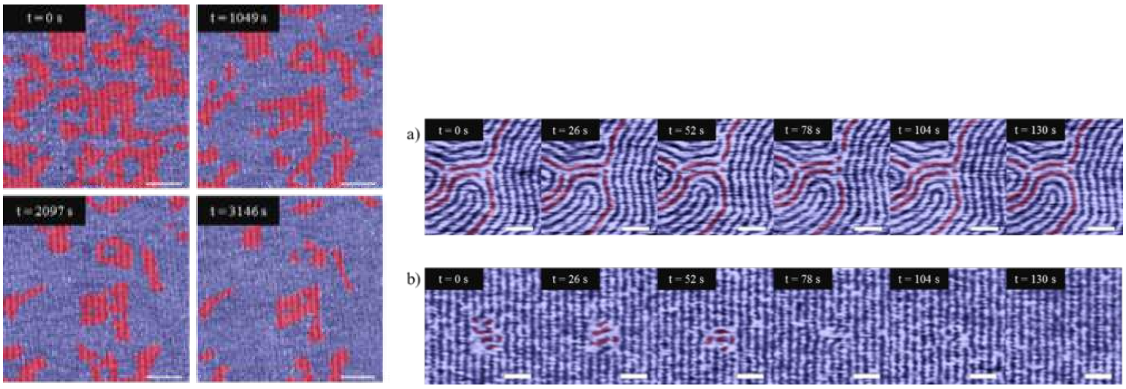


Figure 3.6: Left: AFM images of the *PS-b-PMMA* during in situ thermal annealing. The area fraction of the defective domains were tracked over time to analyze kinetic data. Right: A time sequence of *PS-b-PMMA* on unpatterned substrate during in situ thermal annealing at 210^{o}C shows repeated disconnections and reconnections of strained junctions; in contrast, assembly on chemically patterned substrate shows the irreversible conversion of a stitched domain to aligned lamella.

of defective structures. We observe that domain ordering is mediated by the presence of a non-equilibrium "stitched" microphase morphology. We monitored the rate that stitched domains converted to aligned lamella, finding an effective kinetic barrier for this process of $340 kJ/mol$. Crucially, in contrast to unpatterned samples, assembly on DSA templates was found to be irreversible; no aligned regions were observed to revert to defective states, Figure 3.6.

Database Development of New DSA Processes. The results presented above highlight the fact that knowledge of Chi parameters and surface interaction energies is essential for development of new DSA processes. With that goal in mind, the Use Case has developed a new data base, "pppdb," that has been generated through automated extraction of information from the published literatures.

The 'χDB' database has been led by **de Pablo** (UC) in collaboration with **Audus** (NIST) and **Foster** (UC/ANL) to implement a hybrid human-computer system that extracts Flory-Huggins parameters from the scientific literature. This approach is based on an ambitious attempt to create a digital handbook using automatic extraction and crowdsourcing. This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Figure 7.7 illustrates the number of polymer-polymer χ values in the database. Preliminary expert assessment showed that the literature-extraction approach is a promising strategy for the χ parameter. The χ DB digital handbook, populated by educating students in polymer science and engineering, is now available for material scientists to use and evaluate at http://pppdb.uchicago.edu/. it is currently being expanded to include other properties of polymers, beyond the χ parameter.

Application of machine learning algorithms have been prevailing in the development of "χ-DB". Using publications marked as 'relevant' and a machine learning software, "χ-DB" database has improved the publication selection process by decreasing the number

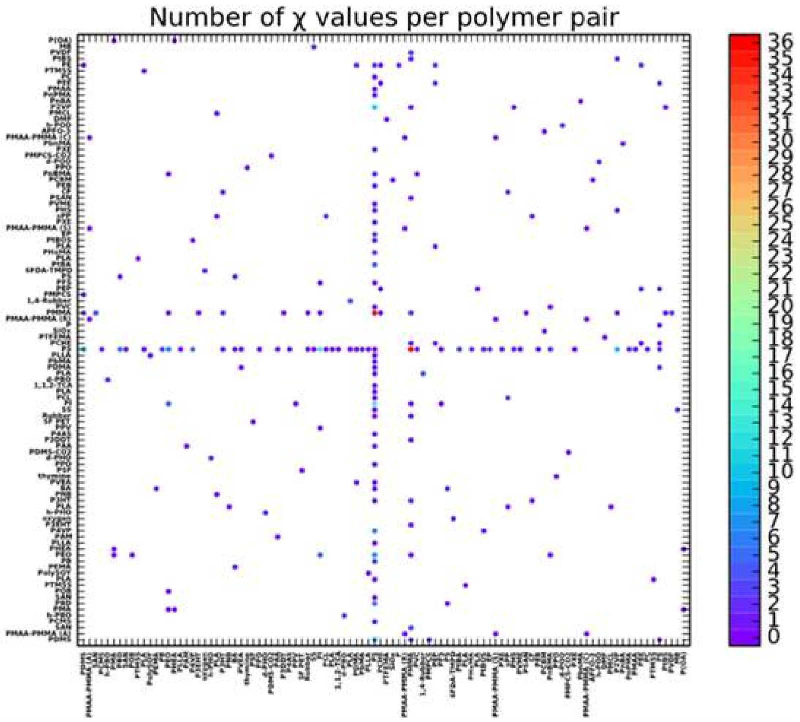


Figure 3.7: Number of χ values per polymer pair

of reviewed publications that do not contribute to the χ database from 60% to 14%. Participation of trained undergraduate students in the curation process has been proven effective in accelerating the data population progress and providing context for ontology development for "χ-DB". Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4].

3.4 Collaborations

3.4.1 CHiMaD Collaborations

3D characterization of block copolymer DSA using X-ray scattering and simulations based reconstruction

Paul ***Nealey*** *(UC), Juan* ***de Pablo*** *(UC)*

The **Nealey** group prepared DSA sample series and performed comprehensive CDSAXS, GISAXS and TEM tomography characterization. The **de Pablo** group developed simulation based data analysis methodology to reconcile information extracted from multiple metrologies into one set of thermodynamic parameters.

Real Time AFM Imaging to Study Kinetics of Block Copolymer Directed Self Assembly

Paul ***Nealey*** *(UC), Steven* ***Sibener*** *(UC)*

The kinetics of microstructure formation on patterned DSA substrates is critical to understanding the origin and fate of metastable defects. High-speed AFM accesses these earliest stages, so one can better assess the processing conditions suitable for fabricating perfected films. CHiMaD-funded graduate students Ren (UC) and Raybin (UC) collaborated to prepare DSA samples and characterize the structural evolution of DSA in real time using high speed AFM.

Material Design Based on Evolutionary Algorithm

*Paul **Nealey** (UC), Heinrich **Jaeger** (UC), Juan **de Pablo** (UC)*

The **Nealey** group collaborated with the **Jaeger** and **de Pablo** groups to develop simulation formulations based on evolutionary algorithm to optimize the DSA processing conditions for desired structures.

3.4.2 NIST Collaborations

3D Characterization of Block Copolymer DSA using CDSAXS

*Joseph **Kline** (NIST), Paul **Nealey** (UC), Daniel **Sunday** (NIST), Juan **de Pablo** (UC)*

Collaborating with the **Kline** group (NIST), CHiMaD-funded graduate student Ren (UC) from the **Nealey** (UC) group prepared DSA samples and performed CDSAXS experiments together with Dr. **Kline** (NIST) during two beam times at the Advanced Light Source at Lawrence Berkeley National Laboratory to characterize the 3D structure of block copolymer. **De Pablo** (UC) performed atomistic simulations of the interfaces to interpret data at the molecular level.

Probing the Interfacial Width of Block Copolymer using Soft X-ray Reflectivity

*Joseph **Kline** (NIST), Daniel **Sunday** (NIST), Paul **Nealey** (UC), Juan **de Pablo** (UC)*

The **Nealey** group (UC) collaborated with **Kline** (NIST) to perform soft X-ray reflectivity measurements at the Advanced Light Source at Lawrence Berkeley National Laboratory in two beam times to study the interfacial width of PS-P2VP as well as PS-PMMA with ionic liquid addition.

Nanoparticle Additives in Block Copolymers

*Jack **Douglas** (NIST), Steven **Sibener** (UC)*

Douglas (NIST) and **Sibener** (UC) groups have ongoing interactions on graphoepitaxy, dynamics of polymer structural evolution, and the effect of nanoparticle additives on local structure in thin polymer films.

Physics Based Interpretation of Scattering Data using Theoretically-Informed Coarse Grain Model

*Joseph **Kline** (NIST), Daniel **Sunday** (NIST), Adam **Hannon** (NIST), Paul **Nealey** (UC), Heinrich **Jaeger** (UC) Juan **de Pablo** (UC)*

Through this collaboration a new formalism that enables interpretation of 3D scattering data for directed self-assembly of block polymers by relying on a physics-based model of the material is being developed. The formalism relies on evolutionary strategies to describe the experimental data, and it is the first of its kind, raising exciting prospects for development of a new generation of metrology tools. Two manuscripts are have been submitted for publication.

TEM Tomography of Block Copolymers

*Jonathan **Winterstein** (NIST), Alexander **Liddel** (NIST), Paul **Nealey** (UC), Juan **de Pablo** (UC)*

The use-case group continued to use the TEM tomography methodology developed together with Winterstein (NIST) and Liddel (NIST) to characterize the 3D structures in various block copolymer DSA systems

Advanced RSoXS Data Analysis Techniques using Self-Consistent Field Theory

*Adam **Hannon** (NIST), Joseph **Kline** (NIST), Daniel **Sunday** (NIST), Paul **Nealey** (UC), Juan **de Pablo** (UC)*

Members of the CHiMaD team and the NIST team are actively collaborating in advanced RSoXS data analysis techniques based on molecular simulations. To this end Adam Hannon (NIST) spent more than six weeks in Chicago working with the **de Pablo** group. Alec Bowen, from the **de Pablo** group, will spend several weeks this summer (2017) at NIST collaborating with **Kline** (NIST) and **Sunday** (NIST).

χ-DB Database
*Debra **Audus** (NIST), Jack **Douglas** (NIST), Ian **Foster** (UC), Juan **de Pablo** (UC), Kenneth **Kroenlein** (NIST)*
Members of CHiMaD and NIST collaborate on development of automated tools for data extraction from the literature and creation of a data base of polymer properties for design of DSA processes. Audus (NIST) spent a month at the University of Chicago in 2015 participating in this collaboration and developing a course on data base creation. As part of this collaboration, a polymer property predictor tool was developed that includes models for homopolymers, copolymers, and charged polymers. Tchoua (UC) visited Kroenlein (NIST) at Boulder to discuss their efforts to extract literature data in the context of thermodynamic fluid properties for process design. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

3.4.3 External Collaborations

3D Characterization of Industry Relevant DSA Processes
*Paul **Nealey** (UC), Paulina Rincon (imec, Belgium), Roel Gronheid (imec, Belgium), Xiaomin Yang (Seagate), Patrick Theofanis (Intel)*
Nealey group collaborated with long-time industry partner at *imec*, *Seagate* and *Intel* to develop metrologies for 3D characterization of industry relevant DSA processes and samples.

Software and Models for Design of DSA *Juan **de Pablo** (UC), Andres Torres (Mentor Graphics)* **De Pablo** collaborated with Andres Torres from Mentor Graphics on development of new tools for simulation of DSA.

Addition of Ionic Liquid for sub-10 nm DSA
*Paul **Nealey** (UC), Takahiro Dazai (TOK, Japan), Paulina Rincon (imec, Belgium), Roel Gronheid (imec, Belgium)*
Nealey group collaborated with *TOK* and *imec* to develop material and processes for sub-10 nm DSA using PS-PMMA with ionic liquid addition.

Complementary 3D Characterization Using Grazing Incidence Small Angle X-ray Scattering and Critical Dimension Small Angle X-ray Scattering
*Paul **Nealey** (UC), Fanny Rodolakis Simoes (ANL), Jessica McChesney (ANL), Zhang Jiang (ANL), Joseph Strzalka (ANL), Jin Wang (ANL), Nicola Ferrier (ANL)*
Nealey group collaborated with researchers from Advanced Photon Source at ANL to develop complementary metrologies for X-ray characterization of block copolymer DSA.

3.5 Technology Transfer

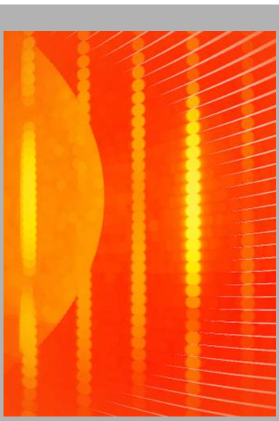
Software
χ-DB Database

J. De Pablo, I. Foster, D. Audus
Link: http://pppdb.uchicago.edu/
This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

3.6 Publications and Presentations

9 Number of CHiMaD-supported publications in 2016 by Directed Self-assembly of Block Copolymer Films for Lithography use-case group. Please see chapter 25 for details. [25.3, 25.4, 25.14, 25.15, 25.16, 25.17, 25.18, 25.19, 25.20]

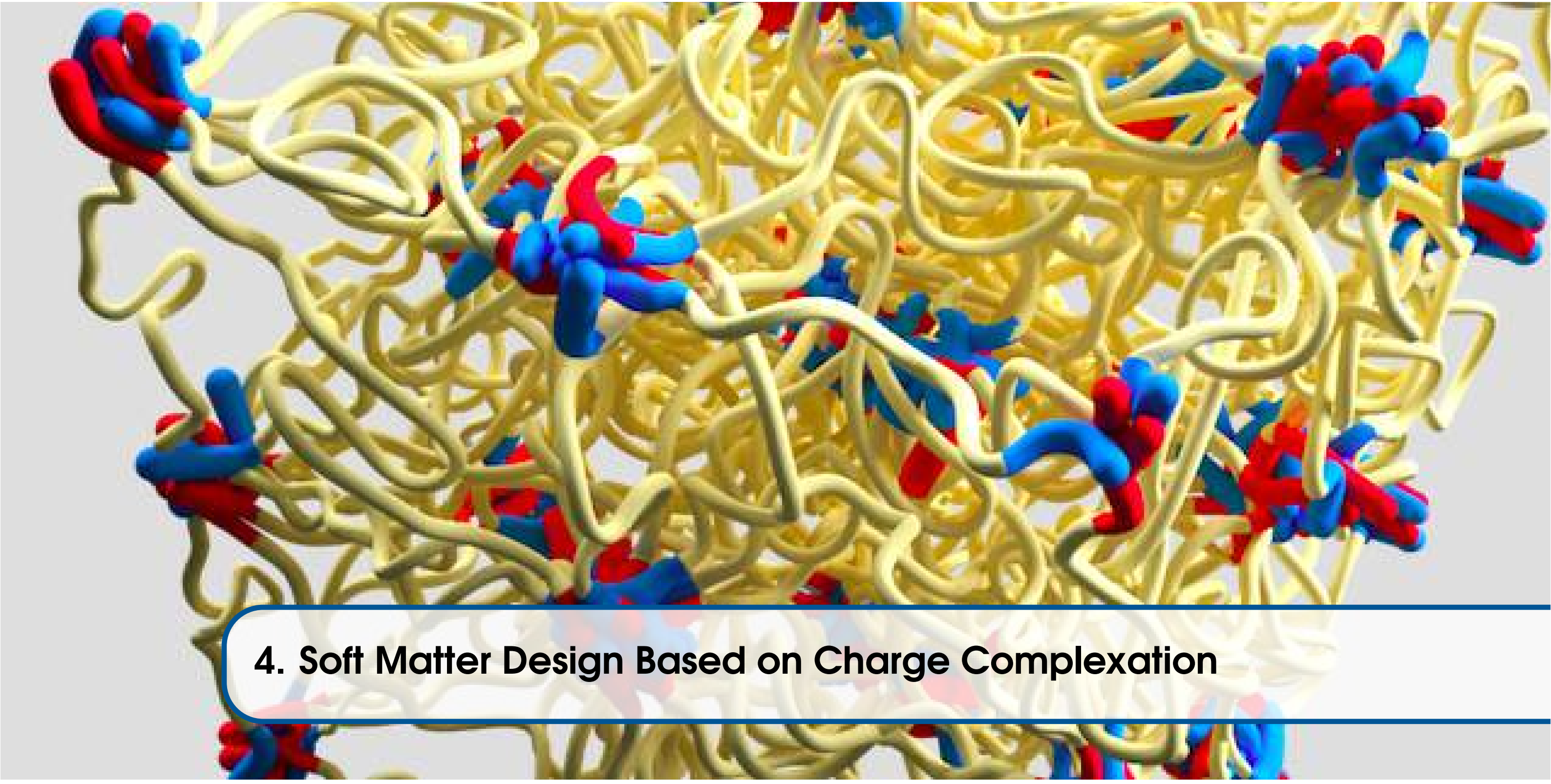
36 Number of presentations on CHiMaD supported research in 2016, please see section 24.3 for the complete list.



Header Image: Resonant soft X-ray scattering aided by molecular simulation reveals the 3D details of block copolymer assembly [Khaira, G. S.; Doxastakis, M.; Bowen, A.; Ren, J.; Suh, H. S.; Segal-Peretz, T.; Chen, X; Zhou, C; Ferrier, N. J.; Vishwanath, V.; **Sunday**, D. F.; Gronheid, R.; **Kline**, R. J.; **de Pablo**, J.J.; **Nealey**, P.F.]

3.7 CHiMaD Team

DSA of Block Copolymers for Lithographic Applications Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Paul Nealey Juan de Pablo Steven Sibener Heinrich Jaeger	Principal Investigator Principal Investigator Principal Investigator Principal Investigator	UC/IME UC/IME UC/CHM UC/PHY	
Manolis Doxastakis	Postdoctoral Researcher	UC/IME	Complementary X-ray characterization using Grazing Incidence Small Angle X-ray Scattering and Critical Dimension Small-Angle X-Ray Scattering *(Nealey)*
Tamar Segal-Peretz	Postdoctoral Researcher	UC/IME	Quantification of block copolymer 3D structures using TEM tomography *(Nealey)*
Hyo Seon Suh	Postdoctoral Researcher	UC/IME	Characterization of 3D structures in block copolymer DSA using GISAXS *(Nealey)*
Jiaxing Ren	Graduate Student	UC/IME	Characterization of 3D structures in the DSA of block copolymer using CDSAXS and TEM tomography *(Nealey)*
Xuanxuan Chen	Graduate Student	UC/IME	Characterization of 3D structures in block copolymer DSA using GISAXS *(Nealey)*
Chun Zhou	Graduate Student	UC/IME	Characterization of 3D structures in block copolymer DSA using GISAXS *(Nealey)*
Endao Han	Graduate Student	UC/PHY	Evolutionary algorithms for materials design of DSA *(Jaeger)*
Leah Roth	Graduate Student	UC/PHY	Evolutionary algorithms for materials design of DSA *(Jaeger)*
Gurdaman Khaira	Graduate Student	UC/IME	Evolutionary algorithms for materials design of DSA *(de Pablo)*
Brandon Peters	Graduate Student	UC/IME	Directed Self-Assembly of Block Copolymers *(de Pablo)*
Roselyne Tchoua	Graduate Student	UC/IME	Creation of chi-parameter Database *(Foster)*
Jonathan Raybin	Graduate Student	UC/CHM	Environmentally controlled AFM of Block Copolymer Directed Self-Assembly *(Sibener)*
Katherine Oosterbaan	Undergraduate Student	UC/CHM	Block Copolymer Membranes for Water Purification *(Sibener)*
Tim Csernica	Undergraduate Student	UC/CHM	Block Copolymer Templates for Organizing Nanomaterials *(Sibener)*



4. Soft Matter Design Based on Charge Complexation

Matthew Tirrell (UC), Juan de Pablo (UC), Monica Olvera de la Cruz (NU), Kenneth Shull (NU), Erik Luijten (NU)

Vivek Prabhu (NIST), Jack Douglas (NIST), Debra Audus (NIST), Kenneth Kroenlein (NIST)

Significance

Soft matter refers to materials where energies of order kT can influence the structure and functions of the materials. One of the main inspirations for soft matter design comes from biology, where many functional materials are built from relatively weak non-covalent interactions. Considerable success has been achieved in creating new materials based on hydrogen bonding and van der Waals interactions. In addition these bonding modalities, and others, biology makes extensive use of electrostatic interactions, frequently mediated by multi-valent ions, including charged polymers. The Use-Case on Soft Matter Design based on Charge Complexation is a comprehensive effort to understand, and employ this understanding to design, new materials based on predictive use of attractive interactions induced by multi-valent interactions in systems of charged polymers. This use-case comprises experimental and theoretical work measuring, simulating and modeling phase diagrams in charged polymer systems, micellization and hydrogel formation in charged block copolymers, and organic inorganic nanocomposites. New materials are being designed and synthesized for biomaterials, drug and gene delivery, bone and tooth repair. This use-case collaborates with Solvay and 3M.

4.1 Design Goals

The integrated goals of this use-case are focused on the *8M program: Molecules, Mixtures, Micelles, Materials, Measurement, Moduli, Modelling, Manufacturing*. This use-case utilizes custom-synthesized macromolecules (M1) to study the phase diagrams of complexation in mixtures (M2) of polyelectrolytes and to exploit the self-assembly possibilities resulting from complexation (M3). Self-assembly via complexation is being used to create micelles, encapsulating materials, coatings, and composite materials (M4). Rheological measurement (M5) gives insight into moduli and other viscoelastic properties (M6). Predictive modelling (M7) of both phase behavior and self-assembly. This fundamental work is input into processing methods (M8) for soft materials based on electrostatic complexation. The **Tirrell** (UC) group seeks, from inputs of macromolecular structure, predictive capabilities into both compositional (e.g., water content) and physical properties (e.g., viscosity, modulus) of complexes formed by charged homopolymer and block copolymers. **Olvera de la Cruz** (NU) continues to develop further a potent self-consistent field approach to the quantitative prediction of phase diagrams in multi-valent polyelectrolyte systems. This work is especially important in capturing the effects of ion correlations on the phase behavior of ion-containing polymers, copolymers and blends. In a parallel effort, the **de Pablo** (UC) group is extending the theoretically informed coarse-grained (TICG) modeling approach, originally developed in the context of neutral block copolymer directed assembly, to charged polymeric materials, including multiblock polymers. The **Shull** (NU) group has invented a novel single step electrochemical self-assembly method, which is being developed to make polyelectrolyte complex (PEC) coatings that have applications as drug delivery vehicles, separation membranes, and biocompatible coatings. **De Pablo** (UC) and **Tirrell** (UC) and co-workers have developed new composite hybrid materials that were prepared by the complexation of gelatin and Laponite (a synthetic silicate in the form of platelets) in aqueous solution followed by carbonization, which hold promise for applications in bone tissue engineering.

4.2 Significant Accomplishments in 2016

Films of polyelectrolyte complex materials **Shull** (NU) group has pursued a new method of creating useful films of polyelectrolyte complex materials. Conventional layer-by-layer (LbL) techniques for polyelectrolyte coatings are low-throughput, multistep processes that are quite slow for building films on the order of micrometers. In this work, PEC films were electrochemically deposited using a rapid one-pot method yielding thick (1μm) films within short experimental time scales (5 min). This rapid electrodeposition was achieved by exploiting the reduction of hydrogen peroxide at the working electrode, triggering the pH responsive self-assembly of a PEC film composed of poly(acrylic) acid and poly(allylamine) HCl. This electrodeposition scheme furthers the development of PEC coatings for more high-throughput applications where a fast and efficient single step approach would be desirable for obtaining conformal coatings, as is the case for electrodeposited paints. This work also introduced a new approach to electrodeposition, one that is potentially more energy efficient while producing high quality polyelectrolyte coatings.

Furthering the fundamental understanding of the structure and pathways of complexation-driven assemblies In a powerful collaboration of experiment and computation, and of CHiMaD with NIST and Oak Ridge National Laboratory, Srivastava (UC), Andreev (UC-NIST), **Prabhu** (NIST), **de Pablo** (UC), and **Tirrell** (UC), along with other co-workers, have elucidated the assembly of oppositely charged triblock copolyelectrolytes into phase-separated gels at low polymer concentrations ($< 1\%$ by mass) via scattering experiments and molecular dynamics simulations. We have shown that, in contrast to uncharged, amphiphilic block copolymers that form discrete micelles at low concentrations and enter a phase of strongly interacting micelles in a gradual manner with increasing concentration, the formation of a dilute phase of individual micelles is prevented in polyelectrolyte complexation-driven assembly of triblock copolyelectrolytes. Gel phases form and phase separate almost instantaneously on solvation of the copolymers. Furthermore, molecular models of self-assembly demonstrate the presence of oligo-chain aggregates in early stages of copolyelectrolyte assembly, at experimentally unobservable polymer concentrations. Our discoveries contribute to the fundamental understanding of the structure and pathways of complexation-driven assemblies, and raise intriguing prospects for gel formation at extraordinarily low concentrations, with applications in tissue engineering, agriculture, water purification and theranostics. This work has been published in Nature Communications [25.23]. Figure 4.1, taken from reference 25.23 shows that triblock copolyelectrolytes are essentially fully interconnected and percolating throughout the sample at concentrations around 0.3% by mass.

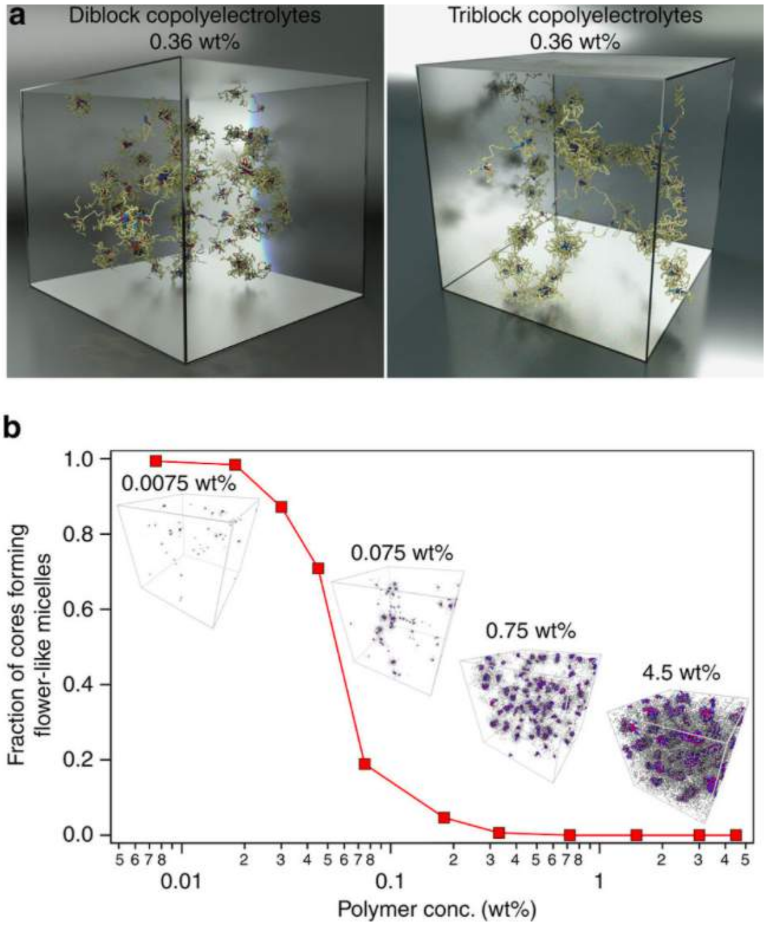


Figure 4.1: TICG Simulations reveal triblock copolyelectrolyte assembly into interconnected gels (a) Snapshots of the simulation box showing self-assembled structures comprising oppositely charged di- and triblock copolyelectrolytes. The polycation, polyanion and neutral blocks are depicted by red, blue and yellow coloured beads, respectively. (b) Fraction of PEC cores forming isolated flower-like micelles as a function of polymer concentration for triblock copolyelectrolyte assemblies. The fraction approaches a near zero value at $\phi = 0.36\%$ by mass. Insets: Snapshots of the simulation box depicting triblock copolyelectrolyte assemblies at various polymer concentrations. The polycation, polyanion and neutral blocks are depicted by red, blue and grey coloured beads, respectively.

A schematic image of the difference in assembly processes between diblock and triblock copolymers is shown in Figure 4.2. The consequences for the rheology and processing behavior of these materials are major; the dynamics of assembly are much slower for triblocks and the viscosity and loss moduli are much higher.

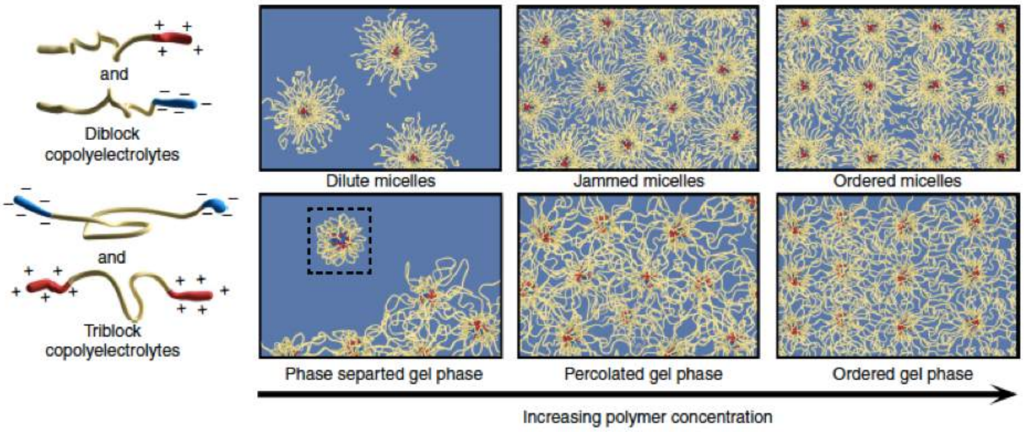


Figure 4.2: Structure evolution of complexation-driven assemblies. Diblock copolyelectrolytes assemble into star-like micelles. At low polymer concentration, discrete micelles remain suspended in the solution. With increasing polymer concentration, micelles jam, thus forming viscoelastic solids, and eventually order in cubic lattice structures. Triblock copolyelectrolytes are expected to form flower-like micelles at extremely low concentrations (the expected flower-like micelle is shown in the inset), but instead form interconnected gels that phase separate from the solution. Increasing polymer concentrations leads to growth of the networks until they percolate through the solution resulting in viscoelastic solids, followed by a disorder-order transition of the PEC domains. In the corresponding jammed/percolated and ordered phases, PEC domains have very similar size and arrangements, leading to nearly identical scattering patterns.

Furthering the fundamental understanding of the structure and pathways of complexation-driven assemblies In another CHiMaD - NIST collaboration, **Douglas** (NIST), along with Andreev (UC-NIST), **Tirrell** (UC) and **de Pablo** (UC), a coarse-grained model of the polymers and the corresponding counter-ions is proposed. The model is used to simulate coacervation as a function of polymer length and overall salt concentration. The results of simulations in different ensembles reproduce a number of phenomena observed in experiments, including the destabilization of the coacervate region by increasing ionic strength or by decreasing molecular weight. The results of the model are also shown to compare favorably with experimental measurements of dynamic modulus. This work has been submitted to ACS Macro Letters, *Complex coacervation in polyelectrolytes from a coarse-grained model*, by Andreev (UC-NIST), Qin (UC), Douglas (NIST), Tirrell (UC), and de Pablo (UC). This theoretical and computational work connects with experimental work in the **Shull** (NU) and **Tirrell** (UC) laboratories that is described in Research Accomplishments section.

Accurate boundary-element method for dielectric anisotropic particles The **Luijten** has improved the iterative dielectric solver with preconditioning techniques for systems with multiple dielectric contrasts.This enables accurate and efficient simulation of dielectrically anisotropic particles, such as proteins and polyelectrolytes, and thus the consequences for predictive properties for complexation, coacervation, and other forms of self-assembly are manifold. As a proof of principle, dielectric effects on the electric double layer of Janus colloids and patchy colloids under electric fields have been studied. Our findings open

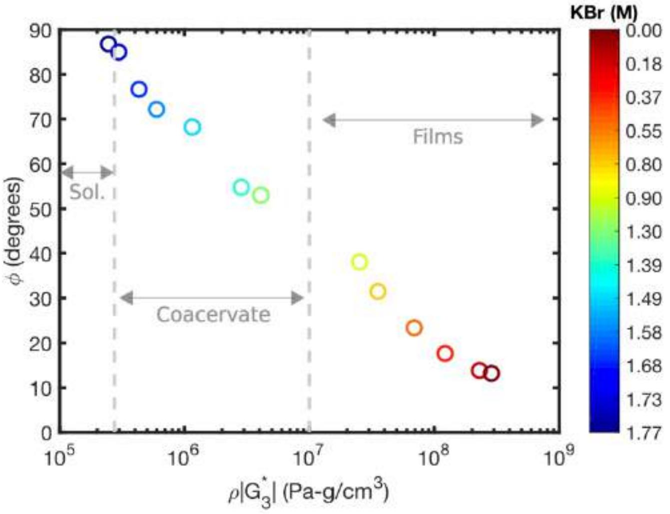


Figure 4.3: The mechanical response of a polyelectrolyte complex composed of polystyrene sulfonate and poly(diallyldimethyl chloride) (PSS:PDADMAC) as a function of salt concentration. The quartz crystal microbalance was used to quantify the continuum of mechanical properties assumed by PSS:PDADMAC, elucidating the transition from films to coacervate to a single phase solution.

pathways toward predictive capabilities for polarizable building blocks for the assembly of new materials. This research was published in Soft Matter [25.9] and Eur. Phys. J. Special Topics [25.8].

4.3 Research Accomplishments

Polyelectrolyte complexes as functional materials. **Shull** (NU) group is working to realize the full potential of polyelectrolyte complexes as functional materials. In this effort, the molecular level details need to be clearly correlated with their dynamic material response. **Shull** (NU) group addresses this issue in two ways: (a) by using the quartz crystal microbalance as a novel rheological technique capable of quantifying the entire mechanical spectrum assumed by polyelectrolyte complexes using poly(styrene sulfonate) and poly(diallyldimethyl chloride) (PSS:PDADMAC) as a model system (see figure 4.3) and (b) by introducing a new model system of alkylated poly(4-vinylpyridine) and poly(styrene sulfonate) (a-P4VP:PSS) whose chain chemistry can be easily modified to probe new insights behind the complexation phenomenon. The versatility of the a-P4VP:PSS system is elucidated by quantifying the effect of side groups and the charge density on the parent chain on complexation, thereby relating chain architecture to the macroscopic material response.

This molecular picture will not only aid the development of stimulus responsive "smart" materials, but also enhance understanding complexation in more challenging contexts, such as in DNA-polymer complexes.

Comparison of Experiment to Theory. In an effort to have a clean experimental system to compare with theory, the **Tirrell** (UC) group, led by graduate student Li, has been studying the phase diagram for polyelectrolyte complexes between polypeptides. The advantages of this system include the fact that the two polymers have identical backbones, and they can be synthesized in the **Tirrell** (UC) laboratory to have very narrow molecular weight distributions. Recent data are summarized in the Figure 4.4. The most striking result from these data are the negative slopes of the tie lines, especially near the critical point in salt concentration on the vertical axis, which is a significant, qualitative departure from the classical Voorn-Overbeek theory, but is captured correctly by the **Douglas** (NIST) - Andreev (UC-NIST) - **de Pablo** (UC) work recently submitted and described above. As these data are quite recent, detailed comparison with theory is just underway. Studies have also been extended to polyelectrolyte pairs to include polymers that also have significant hydrophobic interactions, to see what types of deviations in the phase behavior these interactions produce.

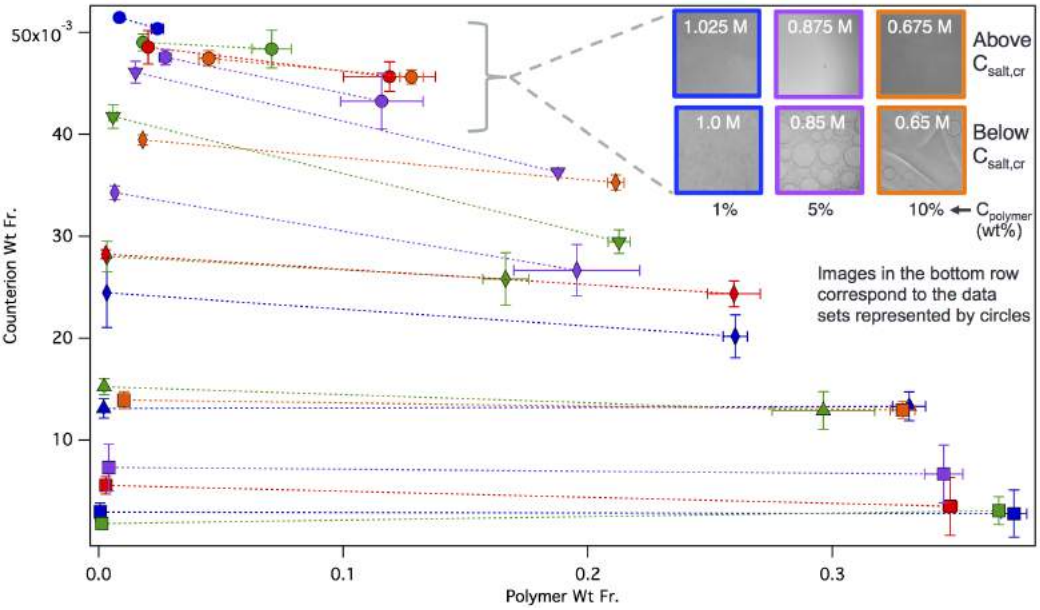


Figure 4.4: Counterions-polymer phase diagram for associative phase separation between polylysine and polyglutamic acis at various polymer concentrations and added salt concentrations

Understanding the electrostatic interactions in copolymers and blends. The **Olvera de la Cruz** (NU) group has been focused on understanding the electrostatic interactions, specifically ionic correlations, ion-containing copolymers and blends. In CHiMaD year three, the group has expanded their model to include the effects of added salt on the miscibility of polyelectrolyte blends and selectivity of the salt. By using liquid state theory and a free energy analysis of ternary polymer blends, we have mapped phase behavior of strongly correlated charged ternary polymer blends. Furthermore, by utilizing SCFT, **Olvera de la Cruz** (NU) group have been able to show that ionic correlations can play a key effect on the selectivity of added salt, where the competitive effects of counterion entropy and ionic correlations can govern the selective swelling of de-swelling of the charge-dense phase in a macroscopically phase-separated polyelectrolyte blends.

’χDB’ database. The ’χDB’ database has been led by **de Pablo** (UC) in collaboration with **Audus** (NIST) and **Foster** (UC/ANL) to implement a hybrid human-computer system that extracts Flory-Huggins parameters from the scientific literature. This approach is based on an ambitious attempt to create a digital handbook using automatic extraction and crowdsourcing. This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers,

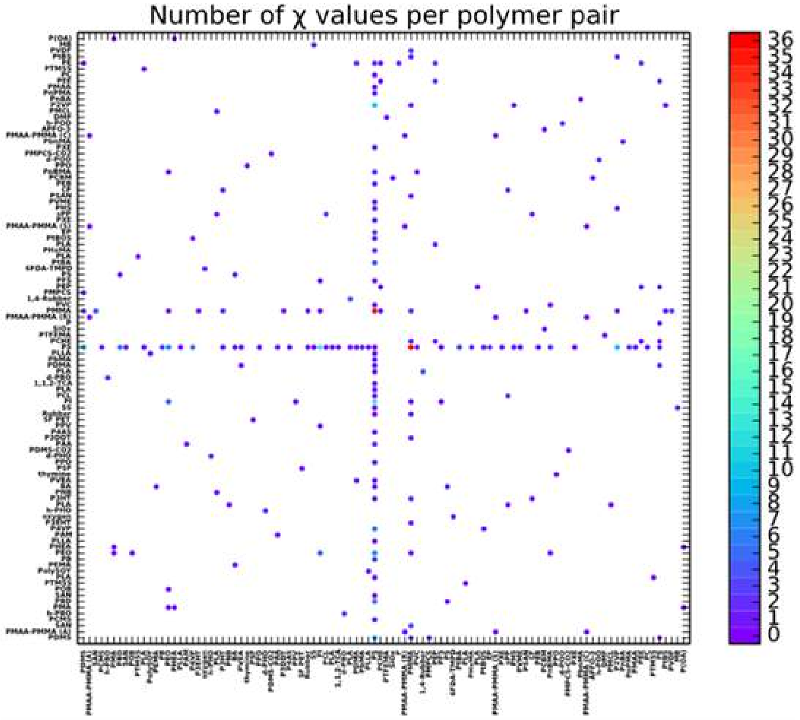


Figure 4.5: Number of χ values per polymer pair

which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Figure 7.7 illustrates the number of polymer-polymer χ values in the database. Preliminary expert assessment showed that the literature-extraction approach is a promising strategy for the χ parameter. The χ DB digital handbook, populated by educating students in polymer science and engineering, is now available for material scientists to use and evaluate at http://pppdb.uchicago.edu/. it is currently being expanded to include other properties of polymers, beyond the χ parameter.

Application of machine learning algorithms have been prevailing in the development of "χ-DB". Using publications marked as 'relevant' and a machine learning software, "χ-DB" database has improved the publication selection process by decreasing the number of reviewed publications that do not contribute to the χ database from 60% to 14%. Participation of trained undergraduate students in the curation process has been proven effective in accelerating the data population progress and providing context for ontology development for "χ-DB". Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4].

4.4 Collaborations

4.4.1 CHiMaD Collaborations

ThermoCalc-generated phase diagrams of charged polymers
Monica ***Olvera de la Cruz*** *(NU), Gregory* ***Olson*** *(NU)*
This collaboration focuses on building a charged polymer database in ThermoCalc for a more robust calculation of equilibrium and metastable phases.

Phase behavior of polyelectrolyte complexes
Monica ***Olvera de la Cruz*** *(NU), Kenneth* ***Shull*** *(NU), Juan* ***de Pablo*** *(UC)*
This collaboration is focused on modeling the partitioning of polyelectrolytes in complexation using LS-SCFT and using TICG models.

All-Polymer Solar Cells
Monica ***Olvera de la Cruz*** *(NU), Tobin* ***Marks*** *(NU)*
Olvera de la Cruz (NU) group performs simulations to calculate the optimal polymer blend morphologies to supplement **Marks** (NU) groups experiments in an effort to increase all-polymer solar cell efficiency.

Polyelectrolyte Assembly
Juan ***de Pablo*** *(UC), Matthew* ***Tirrell*** *(UC)*
This collaboration focused on the characterization and prediction of multi-block polyelectrolyte assembly at low concentrations. This collaboration also examined the rheology of polyelectrolyte assemblies.

4.4.2 NIST Collaborations

Coarse-grained Model for Simulation of the Phase Behavior of Polyelectrolytes
Jack ***Douglas*** *(NIST), Juan* ***de Pablo*** *(UC), Matthew* ***Tirrell*** *(UC)*
Through this collaboration a coarse-grained model for simulation of the phase behavior of polyelectrolytes was developed that includes an explicit description of solvent and ions. The model is the first to be able to describe complex coacervation in polymeric systems. A manuscript is being prepared for submission for publication.

Furthering the fundamental understanding of the structure and pathways of complexation-driven assemblies
Vivek ***Prabhu****(NIST), Juan* ***de Pablo*** *(UC), Matthew* ***Tirrell*** *(UC)*
This collaboration was highlighted in significant accomplishments section, and resulted in a joint NIST-CHiMaD publication in Nature Communcations [25.23]. The discoveries of this NIST-CHiMaD collaboration not only contributes to the fundamental understanding of the structure and pathways of complexation driven assemblies, but also raise intriguing prospects for formation of gel structures at extraordinarily low concentrations, with applications in tissue engineering, agriculture, water purification and theranostics.

Physics-based materials genome for the design of non-equilibrium electrochemical transport processes in polymer membranes for metal-ion batteries
Christopher ***Soles*** *(NIST), Monica* ***Olvera de la Cruz*** *(NU), Juan* ***de Pablo*** *(UC)*
The goal of this collaboration is to design new polymer membranes for batteries. To do so, **Olvera de la Cruz** (NU), Pryamitsyn (NU), **de Pablo** (UC) and Soles (NIST) will develop and apply multi-scale modeling models and methods of non-equilibrium electrochemical transport processes, and will develop new data bases based on such models. By combining machine learning and sophisticated evolutionary computational algorithms with high-information content scattering experiments, the team will generate databases that will accelerate the development and deployment of ion containing polymer membranes for metal-ion batteries.

χ-DB Database
Debra ***Audus*** *(NIST), Ian* ***Foster****, Juan* ***de Pablo*** *(UC), Matthew* ***Tirrell*** *(UC), Kenneth* ***Kroenlein*** *(NIST)*

Members of CHiMaD and NIST collaborate on development of automated tools for data extraction from the literature and creation of a data base of polymer properties for design of DSA processes. Audus (NIST) spent a month at the University of Chicago in 2015 participating in this collaboration and developing a course on data base creation. As part of this collaboration, a polymer property predictor tool was developed that includes models for homopolymers, copolymers, and charged polymers. Tchoua (UC) visited Kroenlein (NIST) at Boulder to discuss their efforts to extract literature data in the context of thermodynamic fluid properties for process design. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

4.4.3 External Collaborations

Block Copolymer-Based Polyelectrolytes
Kenneth ***Shull*** *(NU), Wei Chen (ANL)*
This collaboration focuses on synthesizing model polyelectrolyte systems with well controlled architectures.

Design of Aqueous Based Polyelectrolytes for Consumer Applications
Juan ***de Pablo*** *(UC), Matthew* ***Tirrell*** *(UC), Jean-Yves Delannoy (Solvay)*
This collaboration seeks to design cellulose based high molecular weight polymers to be used in consumer products. The collaboration also involves neutron scientists from NIST.

4.5 Technology Transfer

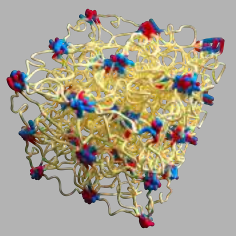
Software
χ-DB Database
J. De Pablo, I. Foster, D. Audus
Link: http://pppdb.uchicago.edu/
This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB digital handbook also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

4.6 Publications and Presentations

9 Number of CHiMaD-supported publications in 2016 by Soft Matter Design Based on Charge Complexation use-case group. Please see chapter 25 for details. [25.3, 25.4, 25.8, 25.9, 25.17, 25.23, 25.24, 25.25, 25.62]

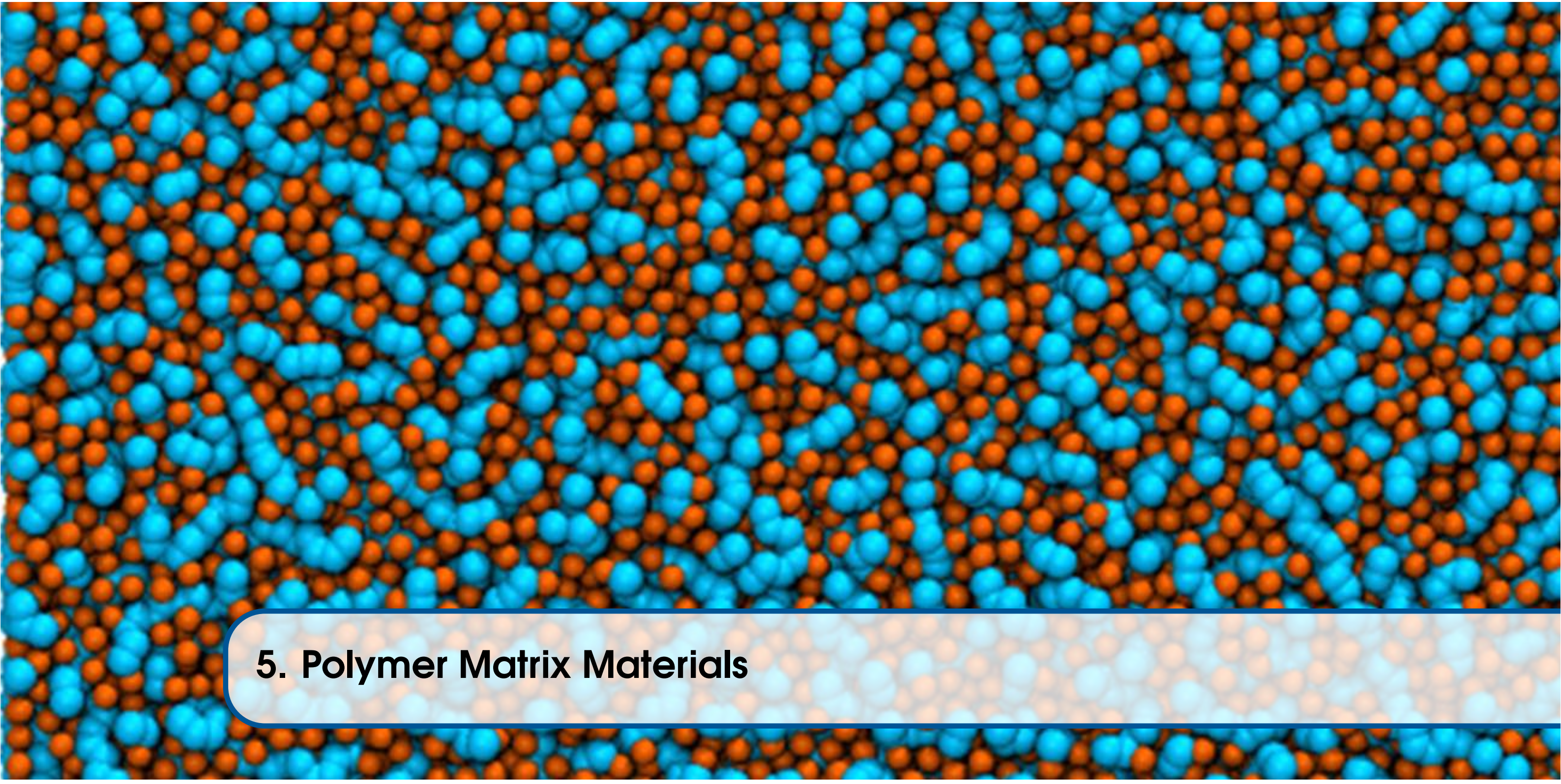
21 Number of presentations on CHiMaD supported research in 2016, please see section 24.5 for the complete list.

4.7 CHiMaD Team



Header Image: A schematic of a hydrogel assembly created from complexation-driven self-assembly of oppositely charged triblock copolyelectrolytes. Authors: Srivastava, Andreev, Levi, Goldfeld, Heller, **Prabhu**, **de Pablo** and **Tirrell**.

Soft Matter Based on Charge Complexation Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Matthew Tirrell Juan de Pablo Erik Luijten Monica Olvera de la Cruz Kenneth Shull	Principal Investigator Principal Investigator Principal Investigator Principal Investigator Principal Investigator	UC/IME UC/IME NU/MSE NU/MSE NU/MSE	
Samanvaya Srivastava	Postdoctoral Researcher	UC/IME	Gel phase formation in dilute triblock copolyelectrolyte complexes *(Tirrell)*
Jeffrey Ting	Postdoctoral Researcher	UC-NIST	Dynamics and molecular mobility in electrostatically self-assembled block copolymers *(de Pablo)*
Marat Andreev	Postdoctoral Researcher	UC-NIST	Polyelectrolyte Complexation *(de Pablo)*
Victor Pryamitsyn	Researcher	NU/MSE	Coarse Grained Simulations of Organic Polymer Solar Cells *(Olvera de la Cruz)*
Ashley Guo	Graduate Student	UC/IME	Biomolecule aggregation and detection *(de Pablo)*
Jiyuan Li	Graduate Student	UC/IME	Biomaterials *(de Pablo)*
Hadi Ramezani-Dakhel	Graduate Student	UC/IME	Biomaterials *(de Pablo)*
Ha-Kyung Kwon	Graduate Student	NU/MSE	Biomaterials *(Olvera de la Cruz)*
Ming Han	Graduate Student	NU/AP	Dielectric Interfaces *(Luijten)*
Zonghui Wei	Graduate Student	NU/AP	Coarse-grained models for PEI *(Luijten)*
Huanxin Wu	Graduate Student	NU/AP	Computational methods for spatially varying permittivity *(Luijten)*
Kazi Sadman	Graduate Student	NU/MSE	Deposition, Mechanics & Equilibrium Structure of Polyelectrolyte Complexes *(Shull)*
Shawn Chen	Graduate Student	NU/MSE	Creep and Fracture of Polyelectrolyte Films in the Non-liner regime *(Shull)*



5. Polymer Matrix Materials

Catherine Brinson (NU), Wei Chen (NU), Juan de Pablo (UC), Sinan Keten (NU), Erik Luijten (NU)

Jeffrey Gilman (NIST), Frederick Phelan Jr (NIST), Jack Douglas (NIST), Debra Audus (NIST), Kenneth Kroenlein (NIST), Materials Data Curation System Team (NIST)

Significance

While polymer composites are lightweight, corrosion resistant and with tailorable properties, their capabilities are vastly under-utilized due to lack of: 1) understanding of multiphase composite properties under small constituent changes, 2) ability to tailor multiple physical properties simultaneously, and 3) durability predictions for long-term properties under use conditions. Tackling these challenges requires a fundamental understanding of the nature of polymer behavior near interfaces (the interphase) and ability to predict microstructure and its impact on properties. In this use case group, we pursue an integrated approach to to relate macroscale polymer composite behavior to chemical constituent and kinetic behavior, and link these resources to development of high-performance modeling and predictive tools. The research includes experimental investigations mapping local physical properties, simulations and analysis to predict microstructure and interphase formation, and a data analytics approach to curate, visualize, and develop analysis and design tools.

The focus of the Polymer Matrix Materials use-case group is initially on polymer nanocomposites, with a long term vision for traditional and hybrid composites. The key of multiphase polymer response is to understand the interaction of filler particles with the matrix material and to explore the physical properties of the interphase zone. This is accomplished both by experimental efforts and physics-based modeling using Molecular Dynamics (MD) and Monte Carlo (MC) simulations to predict interphase polymer response as a function of confinement, crosslinking density and monomer chemistry. At the same time, the researchers of the Polymer Matrix Materials use-case are assembling the known data into a central resource, which will be used with supervised learning methods to identify overarching trends. Combining the physics based methodology with the curated data and tools will provide an unprecedented ability to develop new predictive models of composite behavior.

5.1 Design Goals

The ultimate goal for the Polymer Matrix Materials use-case is to develop databases, models and tools to enable prediction of hierarchical composite behavior based on constituent components and processing.

In short term this use-case aims to;

- Develop the fundamental understanding of interphase properties in cellulose-polymer nanocomposites
- Develop databases, models, and tools to manipulate and design interphase properties in cellulose-polymer nanocomposites and thus control their bulk physical properties (e.g. diffusion, modulus, T_g)
- Develop design rules to tune properties and control service life (e.g., double interphase modulus and double freeze-thaw cycles)

5.2 Significant Accomplishments in 2016

The polymer matrix materials use case has integrated modeling and experimental work to understand the origins of the interphase in polymer-particle systems, curated data on structure and properties, and developed analysis and design tools for nanocomposite systems. This year, significant strides have been made by the group in developing a comprehensive approach to understand and control nanoparticle dispersion in polymer nanocomposites (PNCs) and influence the properties of the PNCs. Experimental methods involving surfactants and ion-exchange techniques were developed to design the surface chemistry of cellulose nanocrystals (CNCs), which successfully led to dramatic improvements in dispersion characteristics of CNCs in polymer matrices. Changes in CNC dispersion were shown to cause changes in many macroscopic properties such as PNC transparency, glass transition temperature, thermal stability, moisture retention/absorption and failure strength. Molecular Dynamic (MD) simulations established that the increased dispersion was due to the reduction of the CNC-CNC cohesive interaction energy and increase of the CNC-polymer matrix adhesion energy. Similarly, grand-canonical Monte Carlo (GCMC) simulations provided molecular-level insights into the moisture-absorption in PNCs using surface-modified CNCs as well as the patterns in local distribution of water molecules around the CNC particles. Correspondingly, super-resolution fluorescence experiments capable of identifying the local distribution of moisture content around CNC particle and high resolution AFM experiments capable of mapping the local mechanical property gradients around CNC-polymer interfaces (i.e. across the interphase regions) were developed. Synergistic experiments and modeling efforts were undertaken to understand the quantitative accuracy of the AFM-based nanomechanical methods. AFM tests on model nanocomposite samples demonstrated the role of nanoparticle spacing (i.e. dispersion) on the local characteristics of interphase mechanical properties around nanoparticles. Statistical/supervised learning techniques were utilized to develop generic visualization and analyses tools capable of identifying the correlation between nanoparticle dispersion, PNC microstructural features and overall PNC properties, and aiding the development of optimal designs of PNCs with targeted mechanical properties. To enhance the pace of material discovery, two novel data resources are being developed as part of CHiMaD: an elegant data resource collecting Flory-Huggins parameters for polymer blends (χ DB) and a comprehensive data resource curating hundreds of properties and parameters describing PNCs (*NanoMine*). The database development efforts are being coordinated with a common high level vocabulary and implementation that allows evolution and interoperability over time. The speed and efficiency of data curation is being addressed by a semi-automatic data curation approach. Data from the simulations and experiments in the use case, data from the published literature, and open source analytical tools have also been incorporated into the public access MGI resources. These accomplishments represent both fundamental new understanding in polymer physics, development of new open-source data and tool resources, and the foundation for true materials design in this complex arena.

5.3 Research Accomplishments

Data Structures and Databases for Polymers and Composites Polymer matrix composites and nanocomposites (PNCs) are an important class structural and functional materials that are widely used in all walks of life. However, their unique compositional attributes (organic polymer or matrix that is usually physically mixed with an inorganic reinforcing filler phase), render such material systems impossible to be thermodynamically simulated from first principle calculations. This difficulty impacts the inclusion of PNCs into the Materials Genome Initiative (MGI) goal of increasing the pace of materials discovery and deployment. One of the primary objectives of this USE-case group has been to overcome this challenge using a two-fold strategy: (a) Creating a centralized repository of comprehensive PNC processing-structure-property data using data curation from published literature and voluntary information contribution from trusted industrial/academic/journal partners. (b) Development of effective data mining and data analysis toolkits that can search through this repository and identify hitherto unknown parameters controlling the structure-property relationships in PNCs. This strategy is envisioned to enable the research community to directly access data and analysis tools to precisely target existing knowledge-gaps, while also encouraging contributions of data and data-analysis tools developed by the community. This objective has been pursued within the use-case by the **Brinson** (NU), **Chen** (NU) and **de Pablo** (UC) groups in collaboration with NIST colleagues, **Phelan** (NIST), and the Materials Data Curation team (NIST).

Toward this goal, two novel data resources are being developed as part of CHiMaD: an elegant data resource collecting Flory-Huggins parameters for polymer blends, χ*DB* and a comprehensive data resource curating over 200 properties and parameters describing nanocomposites, *NanoMine*.

The 'χDB' database has been led by **de Pablo** (UC) in collaboration with **Audus** (NIST) and **Foster** (UC/ANL) to implement a hybrid human-computer system that extracts Flory-Huggins parameters from the scientific literature. This approach is based on an ambitious attempt to create a digital handbook using automatic extraction and crowdsourcing. This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Figure 5.1 illustrates the number of polymer-polymer χ values in the database. Preliminary expert assessment showed that the literature-extraction approach is a promising strategy for the

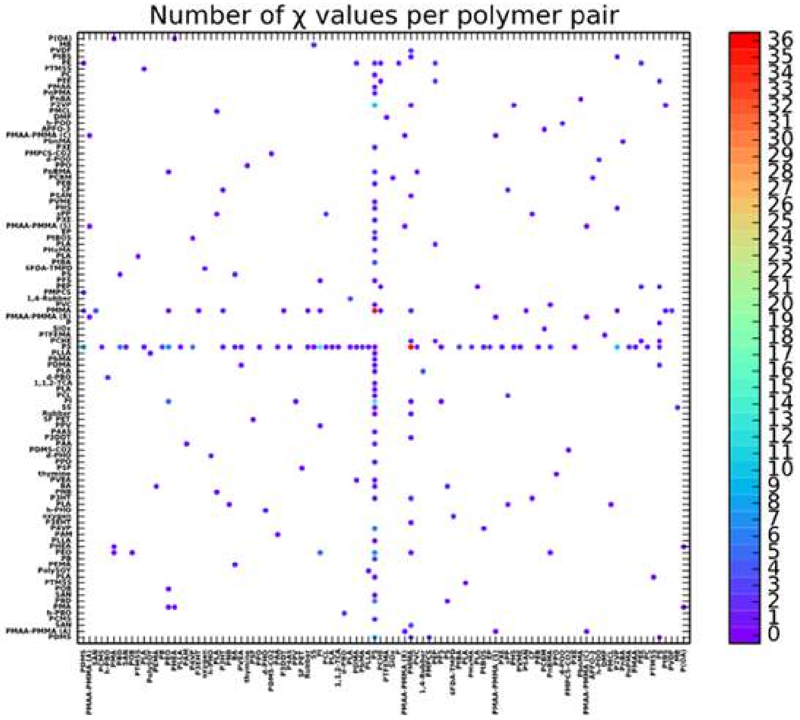


Figure 5.1: Number of χ values per polymer pair

χ parameter. The χ DB digital handbook, populated by educating students in polymer science and engineering, is now available for material scientists to use and evaluate at http://pppdb.uchicago.edu/. it is currently being expanded to include other properties of polymers, beyond the χ parameter.

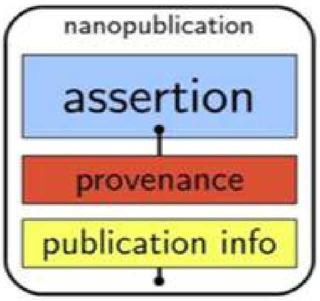


Figure 5.2: All knowledge in *NanoMine* is "nanopublished" to make it easy to access and manipulate publication information and provenance about each knowledge fragment

NanoMine has been developed (**Brinson** (NU), **Chen** (NU) and Zhao (NU)) by customizing the Materials Data Curator (MDC) system developed at NIST with suitable data structures for experimental and computational PNC data and includes three distinct tasks: (i) creation of material data structures (schemas and ontologies) for PNCs, (ii) population/curation of the database with representative sets of PNC data, and (iii) development and integration of data-analytics tools and physics-based modeling tools (**Brinson** (NU), **Chen** (NU) and Li (NU)). *NanoMine* is an ambitious project to track hundreds of different properties and descriptors for nanocomposites, while also accommodating scientific developments through evolving data structures, thus enabling inclusion of emergent parameters downstream. This challenge has been addressed during Year 3 by expanding to an RDF/XML schema that includes extensions for custom data and support for database versioning so that existing documents can be automatically updated to the new schema without data loss or manual intervention. *NanoMine* features a comprehensive nanocomposite material template aiming at tracking more than 200 parameters associated with a given sample. Collaborations with computer science groups (McGuiness (RPI), McCusker (RPI)), have led to the development of a rigorous ontology based on this schema that uses existing standards to encode uploaded data and results as manageable units of experimentally or computationally supported knowledge, called 'Nanopublications'. Updated schema make use of Dublin Core Terms and the BIBO ontology for publication metadata, the Semantic Science Integrated Ontology to represent scientific knowledge, and existing chemical databases like PubChem and PolyInfo to identify chemical entities, thus enabling greater interoperability with existing content. These efforts continue to enable undergraduate summer outreach (Guarino (NU), Ruffenach (NU)) for manual data curation and template refinement. In addition to these manual data curation efforts, currently used by our beta testers, future research efforts (**Brinson** (NU), **Chen** (NU), Wang (NU) and Zhao (NU)) are also underway to automate the data curation process by developing text mining tools to perform large scale topic analysis and data retrieval from online journal publishers. For select publishers, customized crawlers are being created to extract full-text manuscripts and images. Particularly, crawler tools are being set up to automatically retrieve information from five publishers that cover most polymer and composite related journals in order to construct a representative text corpus that can be analyzed with natural language processing and topic modeling techniques.

NanoMine currently includes more than 500 data points from experiments and literature for 20 polymers with 19 types of particles and the data set is continuously expanding with an active team working on data curation from published literature and external curation by colleague beta testers. Existing online material data resources that cover polymers contain a limited number of data for composites. For example, PolyInfo contains data from 1,940 composites in contrast to more than 30,000 pure polymers. Other polymer databases such as Polymers Property Database (CRC) do not contain information on composites. We aim at providing a 'go-to' platform for nanocomposite research and exploration as we continue to work with multiple external collaborators in the scientific and industrial communities to archive lab-generated/published data and implement data-driven tools.

Application of machine learning algorithms have been prevailing in the development of both "χ-DB" and *NanoMine*. Using publications marked as 'relevant' and a machine learning software, "χ-DB" database has improved the publication selection process by decreasing the number of reviewed publications that do not contribute to the χ database from 60% to 14%. For selection of targeted literature in *NanoMine*, curated data from literature serves as training data for machine learning algorithms to better filter and select relevant data to be included. Participation of trained undergraduate students in the curation process has been proven effective in accelerating the data population progress and providing context for ontology development for both *NanoMine* and "χ-DB". Results of our works have been published in Materials Genome special feature of APL Materials, the 2016 International Conference on Computational Science [25.32] and in the Journal for Chemical Education [25.4].

A continuing effort (**Brinson** (NU), **Chen** (NU)) to develop and integrate modular statistical learning tools for characterizing material microstructure and properties into *NanoMine*, has led to the development of a new adaptive optimization based approach for calibration of interphase shift factors. The adaptive optimization based approach is developed to automate and accelerate the search of the interphase properties in polymer nanocomposites to match the simulation output (e.g. permittivity, viscoelastic properties such as dissipation (tan δ), etc.) with experimental data. The approach has been validated for simulation

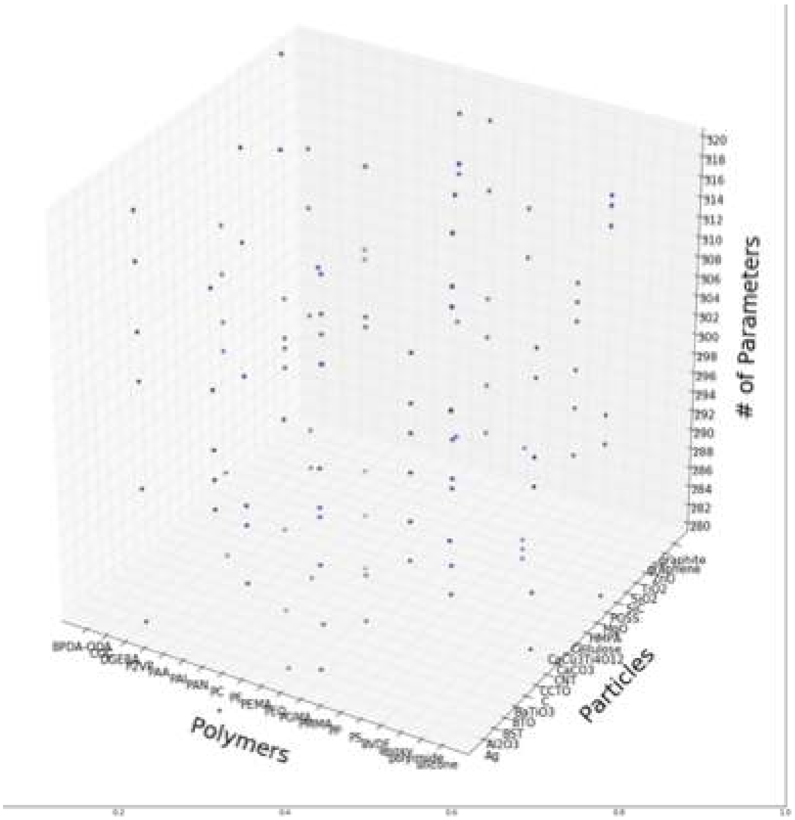


Figure 5.3: Data points in *NanoMine*

models of both dielectric and viscoelastic properties, and improved predictions have been achieved.

During the same time, progress has also been made to utilize previously developed statistical tools such as the *Niblack Binarization* and *Descriptor Characterization* modules to predict structure-property relationships in carbon nanotube (CNT)-based nanocomposites (**Chen** (NU), Li (NU) and Zhang (NU)) in collaboration with NIST (**Gilman** (NIST) and **Davis** (NIST)). Images of CNT composites were characterized with two supervised learning approaches: physical descriptors (e.g., nearest neighbor distance, filler size, etc.) as well as statistical descriptors (e.g., correlation functions, Morishita index and Voronoi diagram), to determine the underlying factors affecting the nanocomposite electrical properties. The extracted characteristics were analyzed to predict CNT's AC and DC conductivities and compared to published data. It was found that cure temperature has significant influence on nanocomposite chemistry and the electrical properties.

Interphase Properties in Polymer Nanocomposites In addition to the individual properties of the matrix and the filler phase, the properties of polymer matrix composites in general and PNCs in particular are greatly dependent on the polymer-filler interaction energy and the dispersion of the filler phase. Chemical and physical interactions between the filler and matrix phases lead to the development of a tertiary bridging "interphase" region. This interphase region has different physical properties than the matrix and are expected to be gradually graded from the filler surface and eventually reach the bulk polymer matrix properties. The property gradient depends strongly on the nature of polymer-filler interactions, but we currently have limited understanding of the factors contributing to the development of the interphase. Therefore, an accurate understanding of the interphase properties (e.g. the interphase length scale) and the relationship between interphase properties and filler-matrix interactions is crucial to accurately predict the properties of PNCs, as well as in the design of PNCs with tailored properties. In this work, we pursue both direct experimental and modeling-based insights into the origins of the interphase mechanical and functional properties.

The Polymer Matrix Materials use-case performs direct AFM and fluorescence based experiments (**Brinson** (NU), **Fox** (NIST), **Gilman** (NIST), Kolluru (NU), Zhang (NU) and Kahraman (NU)) and direct atomistic simulations (**Keten** (NU), **Luijten** (NU), Sinko (NU), Kahraman (NU), Xia (NU/NIST) and Wei (NU)) in conjunction with supervised learning techniques (**Chen** (NU), Li (NU) and Zhang (NU)) to understand various aspects of nanoparticle functionalization, dispersion and interphase development, which will enable tailoring next-generation PNCs with targeted mechanical and functional properties. In the current year, our research efforts have been aimed elucidating: (a) the role of surface modifications (i.e., functionalization) of cellulose nanocrystals (CNC) on their dispersion in a polymer matrix, (b) interactions of water with surface functionalized CNCs and (c) the interphase mechanical property characterization in such material systems.

Surface modification is an effective method to improve the dispersibility of CNCs in the polymer matrix and create nanocellulose/polymer composites that exhibit significant property enhancements. A technique was developed (**Fox** (NIST), **Gilman** (NIST)) using ion exchange resins to replace the sodium ions present on sulphated CNCs with other, larger ions, revealing that replacing sodium ions with ions such as methyl-triphenylphosphonium led to changes in CNC thermal stability, water uptake, and surface energy. Additionally, changing the surface chemistry of the replacement ions led to increased miscibility of the CNCs with nonpolar polymers (epoxy and polystyrene). From a computational perspective, several different ion-exchange surface modifications of cellulose nanocrystals (CNCs) were parametrized (**Keten** (NU)) for use in molecular dynamics (MD) simulations (**Keten** (NU)) and grand-canonical Monte Carlo (GCMC) simulations (**Luijten** (NU)) for their adhesion and moisture adsorption characteristics respectively. The increased dispersion of CNCs in PS-CNC or PMMA-CNC nanocomposites observed in experiments (**Fox** (NIST), **Gilman** (NIST)) was explained by MD simulations (**Keten** (NU)) that provided a dispersion index based on interfacial energies. These simulations revealed that ion exchange surface modifications that confer hyhdrophobicity to CNC surfaces improve dispersion by reducing CNC-CNC cohesion and CNC-amorphous polymer adhesion energy, thus demonstrating the ability to translate nanoscale properties measured using molecular simulations to the bulk properties such as filler dispersion of CNC-amorphous polymer nanocomposites. Similarly, MD simulations of modified CNC-crosslinked epoxy materials systems were used to show that increasing the extent of cross-linking in the epoxy led to a decrease in interfacial adhesion energy. This observation has important implications for considering the trade-off between epoxy mechanical properties and CNC dispersion, and is currently under further investigation. In relation to the materials genome initiative, such MD simulations can be synergistically coupled with the previously described supervised learning techniques (**Chen** (NU)) that can identify the correlation between nanoparticle dispersion, PNC microstructural features and overall PNC properties, to develop optimal designs of PNCs with targeted mechanical properties.

Water/moisture absorption under operating environmental conditions can be detrimental to PNCs structures in many different ways such as disrupting nanoparticle dispersion and

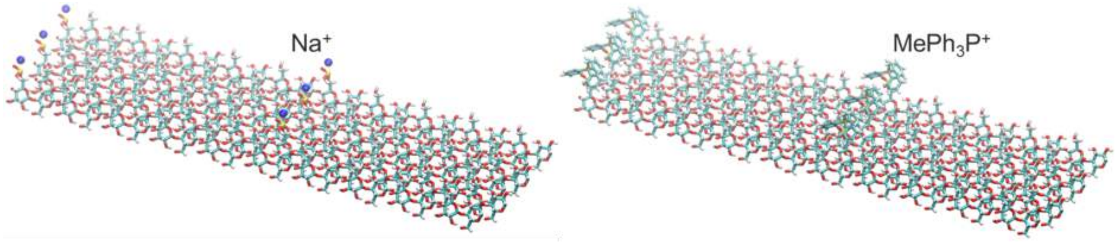


Figure 5.4: *Na*-modified CNC and Methyl(triphenyl)phosphonium ($MePh_3P$)-modifed CNC

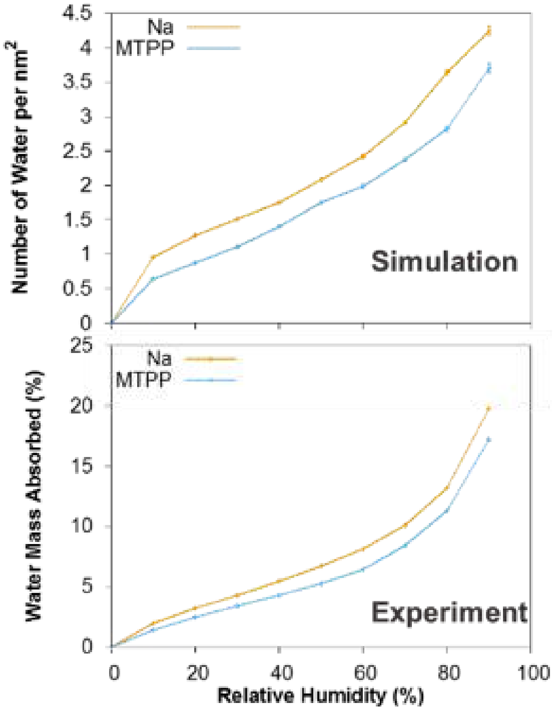


Figure 5.5: The absorbed water mass and surface tension of CNCs with different surface modifications.

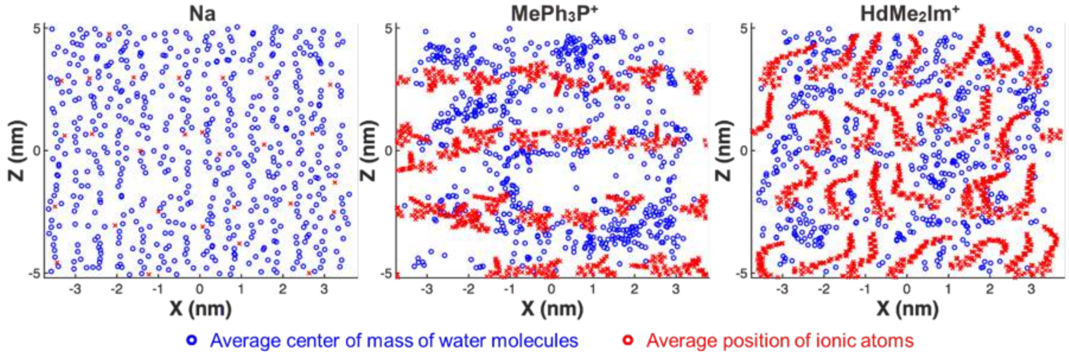


Figure 5.6: Predicted distribution and orientation of water molecules around the ions on the surface of modified CNCs.

affecting the mechanical properties, thus acting as a potential barrier to the successful deployment of PNC structures in harsh environments. The absorbed water mass and surface tension of CNCs with different surface modifications were thus investigated via atomistic CGMC simulations (**Luijten** (NU)) as a function of chemical potential (and thus relative humidity). Trends from simulation results were directly comparable to dynamic vapor sorption experiments (**Fox** (NIST), **Gilman** (NIST)), where the equilibrium absorbed water mass on surface-modified CNCs is measured at different relative humidities, Figure 5.5. The quantitative agreement between simulations and experimental measurements indicated that cation exchange results in reduction in equilibrium water uptake for methyl(triphenyl)phosphonium ($MePh_3P$)-modifed CNC relative to Na-modified CNC. In addition to providing trends that match experimental observations, these simulations were able to provide other molecular insights (**Keten** (NU), **Luijten** (NU)) such as the distribution and orientation of water molecules around the ions on the surface of the modified CNCs, thereby providing the foundation to use simulation in a predictive fashion and speed up materials discovery to design nanocomposites with optimal properties for transportation, infrastructure, and renewable energy applications, Figure 5.6.

Complementary experimental efforts by **Brinson** (NU) have focused on the development of quantitative AFM-based techniques to map the local the interphase mechanical properties. Particularly, model sample geometries (i.e., flat, 1-d samples of amorphous polymer thin film on top of silica slides) have been used to understand the local elastic modulus gradients across the interphase region as a function of physical and chemical interactions. For instance, using such experiments, it has been identified that hydrogen bonding at $PMMA - SiO_2$ interface is shown to increase the interphase length scale. Ongoing experiments are examining effects of cellulose-polymer interactions with the surface functionalities mentioned above. Further experiments (**Brinson** (NU), Kolluru (NU), Zhang (NU)) were performed in collaboration with Torkelson (NU) group at Northwstern University to study the importance of interactions between multiple interphase regions, a precursor to predictively model high volume fraction PNCs. A PS-silicon nanocomposite system shows additional stiffening of the embedded polymer matrix when the distances between the silicon surfaces drops below 200 nm (indicating interaction of interphases), Figure 5.6. These observations complement the studies on nanoparticle dispersion (described earlier), as variance in nanoparticle dispersibility leads to varying inter-particle spacing and thus appropriate interphase characteristics described by the AFM experiments need to be utilized in predictive models. Additional research efforts in this area are focused on a

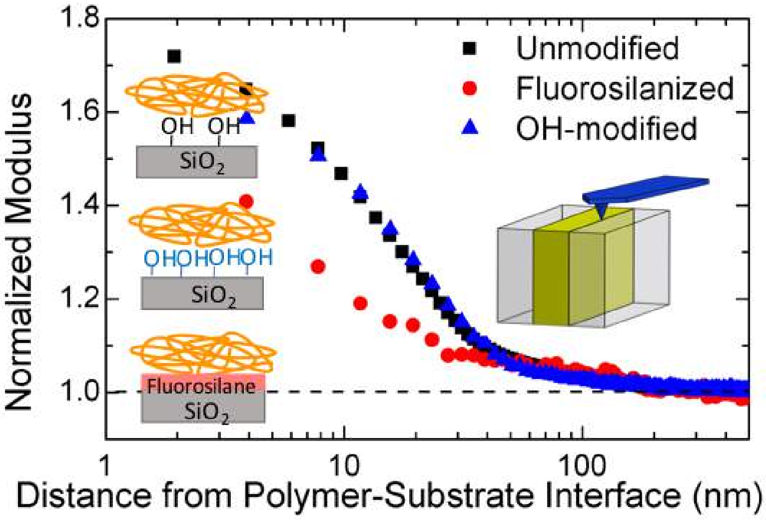


Figure 5.7: Local elastic modulus gradients across interphase region

multiscale understanding of the properties in the interphase regions of PNCs in external collaborations with industrial research partners such as *Dow* (**Keten** (NU)), *Goodyear Rubber and Tire Company* (**Brinson** (NU)) and *Owens Corning* (**Brinson** (NU),**Gilman** (NIST)).

Synergistic experimental (**Brinson** (NU)) and computational (**Brinson** (NU), **Keten** (NU)) research has also focused on ensuring the reliability of quantitative mechanical property data obtained by way of a sensitive instrumented indentation methodology. Current efforts include the development of finite element analysis (FEA) simulations (**Brinson** (NU), Zhang (NU), Kolluru (NU)) that validated recent MD simulation results (**Keten** (NU) and Xia (NU/NIST)) in describing the effects of AFM-tip radius on the measured stress field interaction effects on mechanical properties, Figure 5.8. However, experimental efforts (**Brinson** (NU) and Kolluru (NU)) highlight the challenges of reality: data demonstrates that the interphase length scale in a PS-silica system, are significantly large, on the order of 200 nm and independent of tip-radius artifacts, Figure 5.9. Some of the likely differences between the experiments and modeling efforts are expected to arise from differences in strain rate, temperature and material plasticity, and will be the focus of future work in this area.

5.4 Collaborations

5.4.1 CHiMaD Collaborations

Characterization of Interphase Properties
*Catherine **Brinson** (NU), Sinan **Keten** (NU), Erik **Luijten** (NU)*
The three groups are coordinating experimental (AFM) and modeling (MD) efforts on understanding of interphase properties.

NanoMine Data Resource
*Catherine **Brinson** (NU), Wei **Chen** (NU)*
The two groups are developing the *NanoMine* data resource, models and tools for nanocomposites.

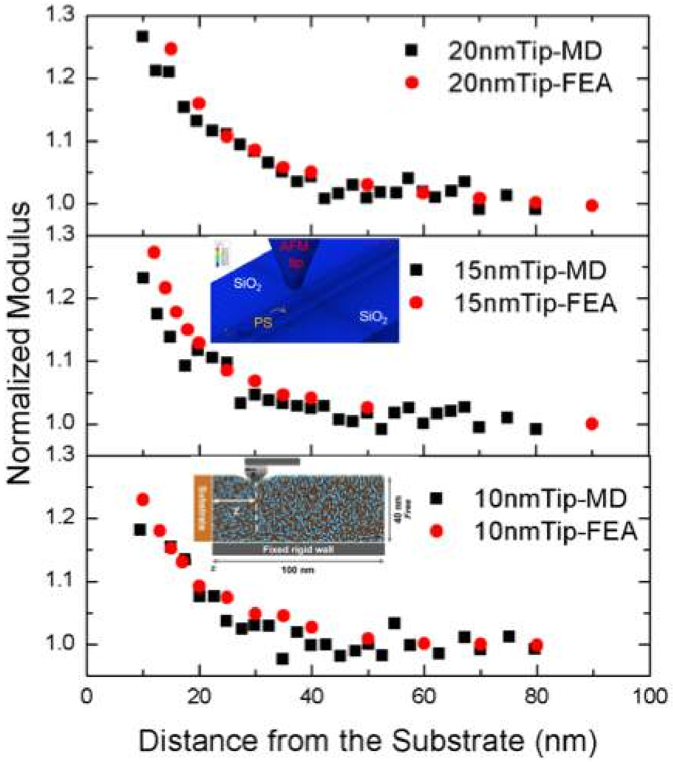


Figure 5.8: Effects of AFM tip radius via MD and FEA confirm impact of substrate stress field interaction

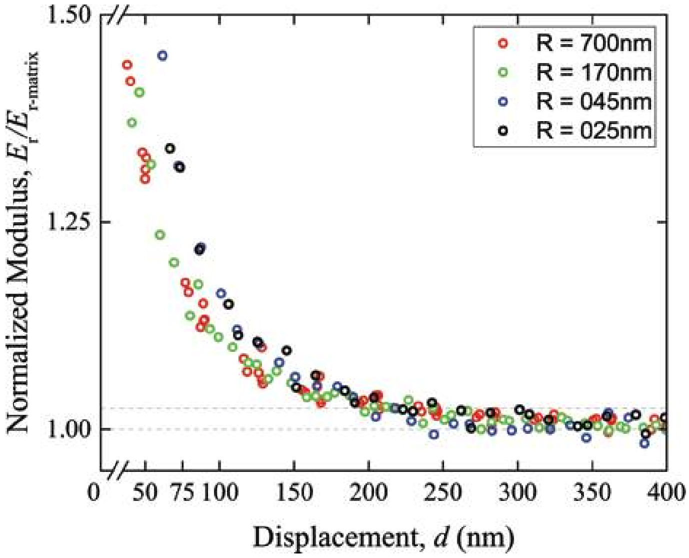


Figure 5.9: Interphase length scale in PS-silica system with substrate stress field interaction removed

Characterization of Moisture Absorption onto Cellulose Nanocrystals

*Sinan **Keten** (NU), Erik **Luijten** (NU)*

Keten group characterized ion-exchange surface modifications of CNCs, to be used in MD simulations as well as GCMC simulations lead by **Luijten** group on moisture absorption onto CNCs.

5.4.2 NIST Collaborations

Characterization of Interphases

*Catherine **Brinson** (NU), Jeffrey **Gilman** (NIST)*

Brinson and Gilman groups collaborated on coordinating AFM and Flourescence experiments in sample preparation and characterization of polymer-particle interactions.

Identification of Key Filler Descriptors for Carbon Nanotubes

*Wei **Chen** (NU), Chelsea **Davis** (NIST)*

In collaboration with **Davis** (NIST), using carbon nanotubes as an illustrative example, **Chen** group will demonstrate the capability of our methods by identifying key filler descriptors from (CNT) experimental images acquired by **Davis** (NIST), to achieve a better understanding of their impact on properties and perhaps correlations with temperature effects. Statistical characterization and machine learning techniques will be applied to characterize the filler structures and study their relations with properties.

Surface Chemistry Effects on Nanocomposite Properties

*Sinan **Keten** (NU), Jeffrey **Gilman** (NIST), Douglas Fox (American University)*

This collaboration will characterize the dispersion of cellulose nano-crystals (CNC) and use MD simulations to predict the impact of key descriptors such as distribution of minimum distance and compare the results with the experiments of T_g and modules measurements. Two different CNCs with different surface energies and loading weights (VF) will be considered.

Coarse-grained Model Development

*Sinan **Keten** (NU), Jack **Douglas** (NIST), Frederick **Phelan** Jr. (NIST)*

This collaboration focuses on systematic coarse-graining of glass forming polymers.

χ-DB Database

*Debra **Audus** (NIST), Jack **Douglas** (NIST), Ian **Foster** (UC), Juan **de Pablo** (UC), Kenneth **Kroenlein** (NIST)*

Members of CHiMaD and NIST collaborate on development of automated tools for data extraction from the literature and creation of a data base of polymer properties for design of DSA processes. Audus (NIST) spent a month at the University of Chicago in 2015 participating in this collaboration and developing a course on data base creation. As part of this collaboration, a polymer property predictor tool was developed that includes models for homopolymers, copolymers, and charged polymers. Tchoua (UC) visited Kroenlein (NIST) at Boulder to discuss their efforts to extract literature data in the context of thermodynamic fluid properties for process design. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

5.4.3 External Collaborations

Nanocomposite Database Development

*Catherine **Brinson** (NU), Wei **Chen** (NU), Linda Schadler (Rensselaer Polytechnic Institute), Deborah McGuiness (Rensselaer Polytechnic Institute), James McCusker (Rensselaer Polytechnic Institute)*

This collaboration focuses on development of ontologies, visualization tools and robust data science infrastructure for *NanoMine* data resource.

Nanocomposite Characterization and Modeling

*Catherine **Brinson** (NU), Wei **Chen** (NU), Linda Schadler (Rensselaer Polytechnic Institute)*

This collaboration focuses on fundamentals for understanding polymer nanocomposite interactions and development of design and analysis tools.

Interphase Properties for Nanocelulose

*Catherine **Brinson** (NU), Douglas Fox (American University/NIST)*

This collaboration focuses on examining the impact of surfaces on polymer interphase. As a part of this collaboration, samples of functionalized cellulose were exchanged.

Local Polymer Characterization

*Catherine **Brinson** (NU), John Torkelson (NU)*

This collaboration involves fundamental work on understanding polymer interactions at interfaces with controlled chemistries along with comparison across experimental methods.

Size-selective Nanoparticle Assembly on Substrates by DNA Density Patterning

*Erik **Luijten**, Vinayak Dravid (NU), Chad Mirkin (NU)*

This collaboration aims to employ molecular dynamics simulations to explore the size-selection behavior of two-dimensional assembly of spherical DNA-modified gold nanoparticles on DNA-grafted substrates. We show that the larger surface coverage by small particles provides a thermodynamic advantage for assembly at high DNA density, but that large particles dominate at low density where small particles cannot access a sufficient number of linkages for immobilization.

Collaborations with The Dow Chemical Company

*Sinan **Keten** (NU)*

This collaboration focuses on determining the reliability and quantitative accuracy of nanoparticle dispersion and interphase size and properties between computational simulations and experiments.

Collaboration with The Goodyear Tire & Rubber Company

*Catherine **Brinson** (NU), Wei **Chen** (NU)*

This collaboration focuses on determining the reliability and quantitative accuracy of nanoparticle dispersion and interphase size and properties between computational simulations and experiments.

Collaboration with Owens Corning

*Jeffrey Gilman (NIST), Catherine **Brinson** (NU), Dave Hartmann (Owens Corning)*

Owens Corning is funding a joint NIST/NU project on quantifying interphase formation in glass-polymer composites based on results from the Polymer Matrix Materials use-case group.

5.5 Technology Transfer

Software
NanoMine
C. Brinson, W. Chen, L. Schadler, R. Zhao, Y. Wang, X. Li
Link: http://NanoMine.northwestern.edu
NanoMine currently can perform basic functionality for data curation (data entry with pre-defined schema) and data exploration (selecting from existing materials and look up data by query). The current beta version is ready for distribution to volunteering academic and industrial research groups for system testing, communal curation and feedback.

Software
χ-DB Database
J. De Pablo, I. Foster, D. Audus
Link: http://pppdb.uchicago.edu/
This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

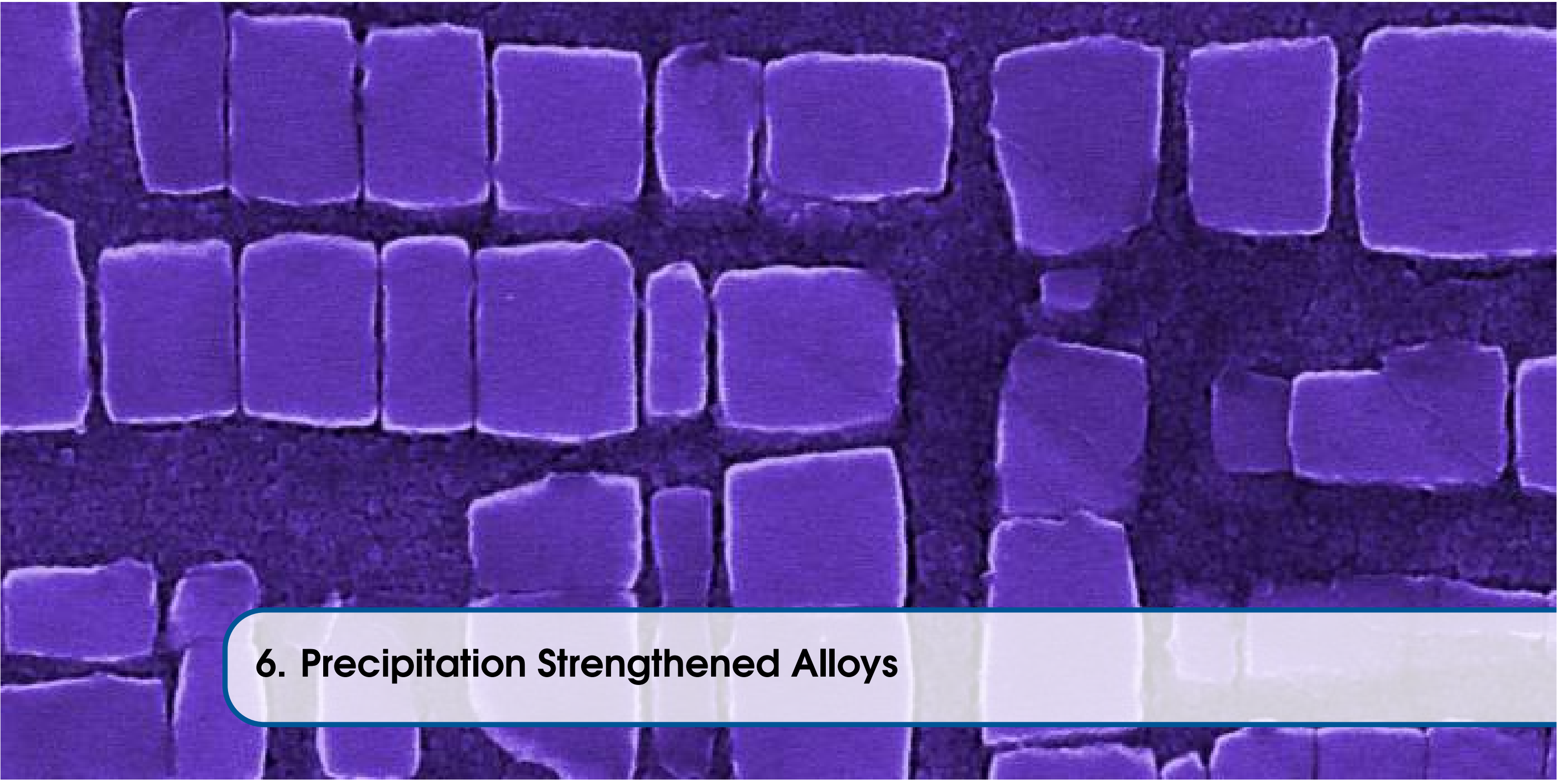
5.6 Publications and Presentations

9 Number of CHiMaD-supported publications in 2016 by Polymer Matrix Materials use-case group. Please see chapter 25 for details [25.1, 25.2, 25.3, 25.4, 25.5, 25.6, 25.7, 25.8, 25.9].

28 Number of presentations on CHiMaD supported research in 2016, please see section 24.2 for the complete list.

5.7 CHiMaD Team

Polymer Matrix Materials Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Catherine Brinson Wei Chen Juan de Pablo Sinan Keten Erik Luijten	Principal Investigator Principal Investigator Principal Investigator Principal Investigator Principal Investigator	NU/ME NU/ME UC/IME NU/ME NU/MSE	
Pavan Kolluru	Postdoctoral Researcher	NU/ME	Local polymer properties via AFM for Nanocellulose-Polymer interfaces *(Brinson)*
Wenjie Xia	Postdoctoral Researcher	NU-NIST	Transferable coarse-grained models for glass-forming polymers *(Keten, Douglas, Phelan)*
Richard (He) Zhao	Graduate Student	NU/ME	*NanoMine* data resource *(Brinson)*
Yixing Wang	Graduate Student	NU/ME	*NanoMine* data resource, data mining and simulations *(Brinson)*
Min Zhang	Graduate Student	NU/MSE	AFM characterization of model nanocomposite interfaces *(Brinson)*
Xiaolin Li	Graduate Student	NU/ME	Microstructure Reconstruction and Analysis *(Brinson, Chen)*
Yichi Zhang	Graduate Student	NU/ME	Microstructure characterization and reconstruction *(Chen)*
Yongri Su	Graduate Student	UC/IME	Nanocomposites *(de Pablo)*
Xin Qin	Graduate Student	NU/ME	Coarse-grained modeling of CN neat films *(Keten)*
Bobby Sinko	Graduate Student	NU/ME	Surface modifications effects on moisture absorption and interfacial properties of CNCs *(Keten)*
Ridvan Kahraman	Graduate Student	NU/MSE	Interphase characterization of CNC nanocomposites with AFM and MD *(Keten, Brinson)*
Huanxin Wu	Graduate Student	NU/PHY	Computational methods for spatially varying permittivity *(Luijten)*
Ryan Franks	Graduate Student	NU/MSE	GPU-based modeling of DNA-coated colloids *(Luijten)*
Valentine Guarino	Undergraduate Student	NU/ME	*NanoMine* data resource curation (Summer Project) *(Brinson)*
Anetta Siemianowicz	Undergraduate Stundent	NU/ME	*NanoMine* data resource curation (Summer Project) *(Brinson)*



6. Precipitation Strengthened Alloys

Gregory Olson (NU), David Dunand (NU), David Seidman (NU), Wei Chen (NU), Christopher Wolverton (NU), Ankit Agrawal (NU), Alok Choudhary (NU), Yip-Wah Chung (NU), Michael Bedzyk (NU), Wing-Kam Liu (NU), A. Umantsev (FSU), Olle Heinonen (ANL), Peter Voorhees (NU), Marius Stan (ANL)

Jason Sebastian (QuesTek), James Saal (QuesTek), David Snyder (QuesTek), Ida Berglund (QuesTek), Dana Frankel (QuesTek), Clay Houser (QuesTek)

Carelyn Campbell (NIST), Ursula Kattner (NIST), Eric Lass (NIST), Shengyen Li (NIST), Kil-Won Moon (NIST), Maureen Williams (NIST), Lyle Levine (NIST), Mark Stoudt (NIST)

Significance

New capabilities in predictive design of precipitation-strengthened alloys are being applied to Co-based superalloys and high-performance Shape Memory Alloys, both employing low-misfit coherent aluminide precipitates closely analogous to the γ*-* γ' *Ni-based superalloys. The Co-based alloys are of interest for both high-temperature creep and fatigue resistance in turbine applications, as well as ambient temperature wear-resistance applications such as aerospace bushings to replace Be-Cu alloys. The shape memory alloys are of high interest for device and actuation applications in medicine, aerospace and automotive sectors where ultrahigh-cycle fatigue is the primary limitation of current alloys; here, efficient precipitation strengthening can eliminate the accommodation slip associated with thermoelastic martensitic transformation, standing as the principal cause of cyclic instability.*

6.1 Design Goals

New capabilities in predictive design of precipitation-strengthened alloys are being applied to Co-based superalloys and high-performance Shape Memory Alloys, both employing low-misfit coherent aluminide precipitates closely analogous to the $\gamma - \gamma'$ Ni-based superalloys.

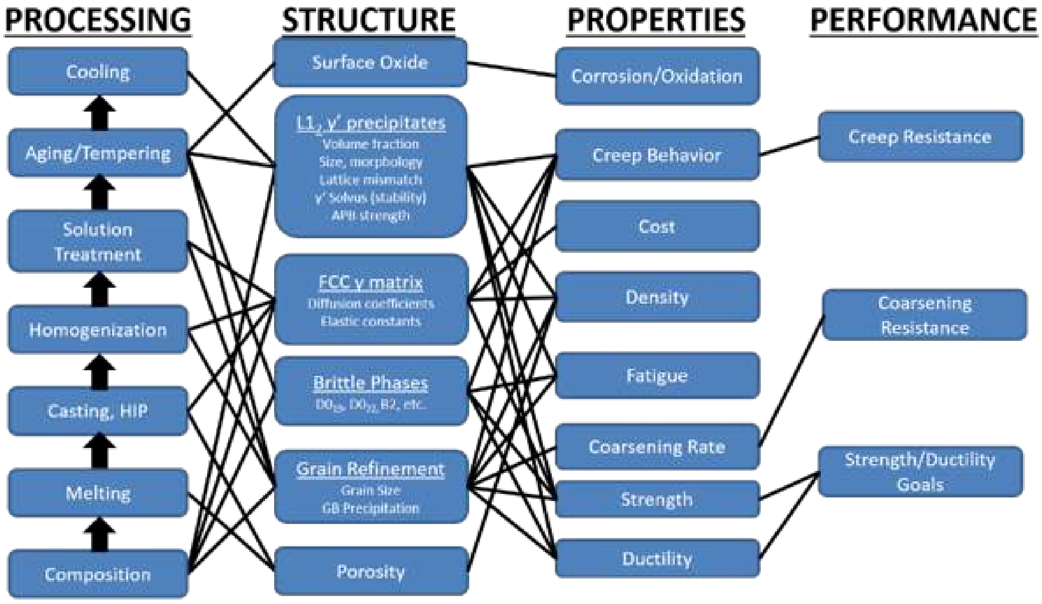


Figure 6.1: Systems design chart of Cobalt Superalloys

The Co-based alloys are of interest for both high-temperature creep and fatigue resistance in turbine applications, as well as ambient temperature wear-resistance applications such as aerospace bushings to replace Be-Cu alloys. The shape memory alloys are of high interest for device and actuation applications in medicine, aerospace and automotive sectors where ultrahigh-cycle fatigue is the primary limitation of current alloys; here, efficient precipitation strengthening can eliminate the accommodation slip associated with thermoelastic martensitic transformation, standing as the principal cause of cyclic instability.

Short-term goals for the Co alloys address ambient temperature applications, where the intrinsic low surface friction characteristics of Co-based alloys makes their precipitation strengthened variants of clear near-term interest as a replacement for Be-Cu aerospace bushing applications of current environmental concern. Long-term goals address high-temperature applications (represented by the system chart of Figure 6.1) where metallic superalloys play a vital role in electrical power generating systems (gas and steam turbines) and jet engines. While achievement of the full set of properties necessary for these applications is an ambitious goal, the potential of the new family of Co-based superalloys to achieve the same strength levels of current Ni-based superalloys, but with a temperature capability $100-150^{o}C$ higher would enable a major advance in the fuel efficiency of gas turbines and jet engines. In support of new capabilities in additive manufacturing by 3D printing, precipitation-strengthened superalloy research also addresses processability constraints to design alloy variants compatible with the new manufacturing processes.

The breadth of developing databases for Shape Memory alloy design support both the near-term optimization of high Pd alloys for medical applications favoring high radiopacity and low Ni content for biocompatibility (Figure 6.2), and the longer-term design of lower-cost high Zr alloys to meet the requirements of aerospace and automotive actuators. This will allow the new class of cyclically-stable alloys to have broad technological impact.

A further extension of our precipitation-strengthening research in the past year has been

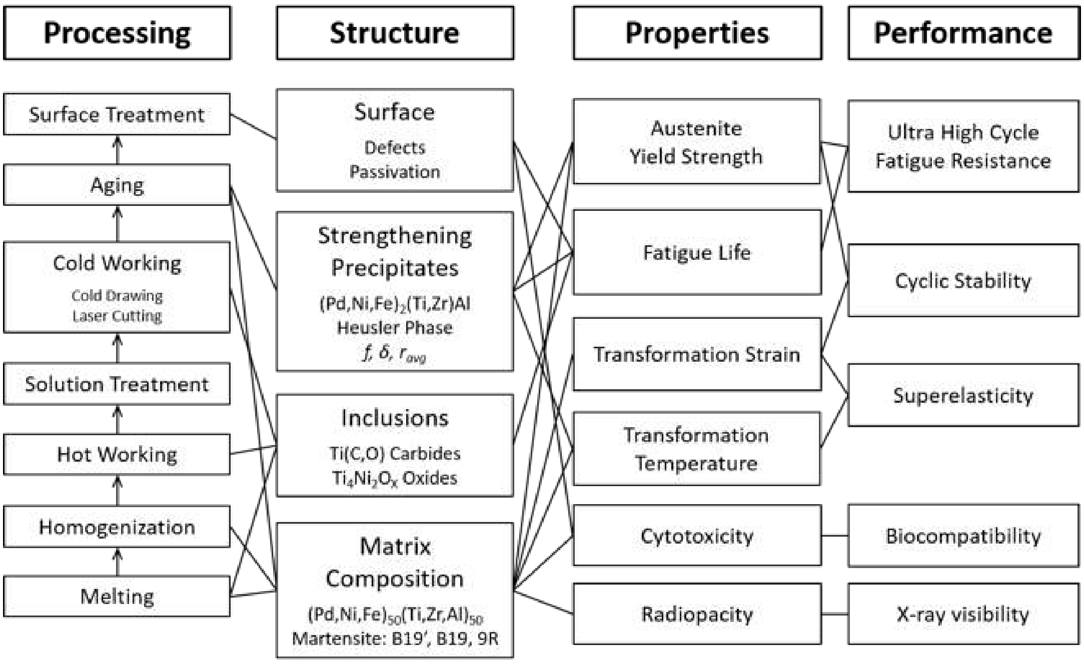


Figure 6.2: Systems design chart of High-Performance Shape Memory Alloys

application of the same precipitation principles to management of thermal conductivity in multiphase thermoelectric materials under the DARPA SIMPLEX program.

6.2 Significant Accomplishments in 2016

During 2016, Precipitation-Strengthened Alloys use-case group researchers have concentrated on building on their results from previous years and advancing the field in the following topics:

- Experimentation for Co-alloy fundamental data development
- Co-Based CALPHAD Database Development
- High-throughput Combinatorial Synthesis
- DFT Calculations of Diffusion in Co and Interfacial energies
- High-Performance Shape Memory Alloys
- Fatigue Nucleation Modeling
- Industrial Accelerated Qualification of Materials - Co-alloy development
- Industrial Accelerated Qualification of Materials - Shape memory alloy development
- Precipitation-Strengthened Thermoelectrics and CALPHAD development
- Steel Research Group (SRG) Projects and Design Class Interactions

A detailed explanation of research achievements in each topic can be found in the next section.

6.3 Research Accomplishments

Experimentation for Co-alloy fundamental data development In collaboration with **Lass** (NIST), the effects of Cr additions for high temperature oxidation resistance in multinary Co-based superalloys are currently being assessed by Chung (NU) from the **Dunand** and **Seidman** groups. Multiple Cr-containing alloys were arc-melted at NIST to examine the

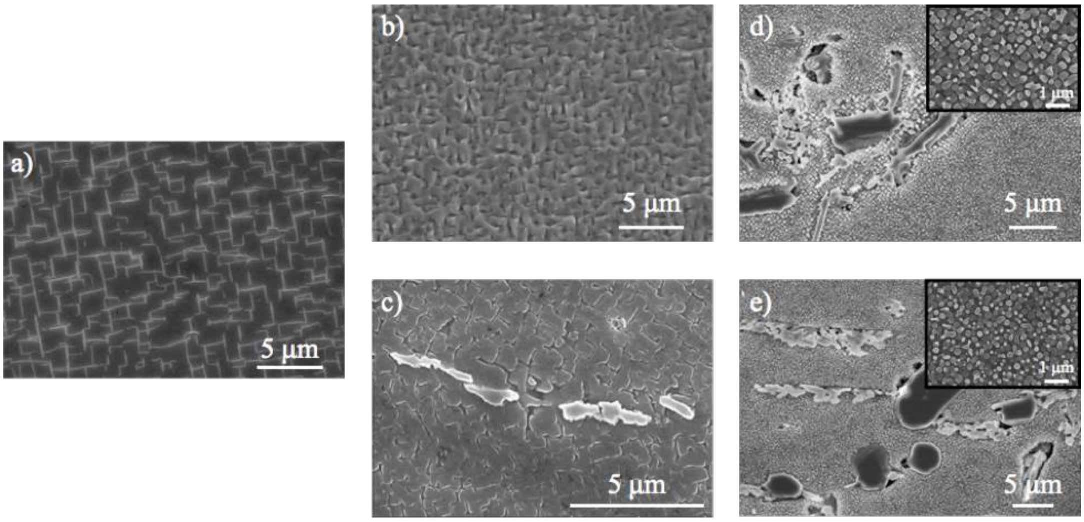


Figure 6.3: Secondary electron SEM micrographs of Co-Ni-Al-W-Ti-Ta-Cr alloys aged at 900°C for 168h with: a) 0 at% Cr, b) 4 at% Cr, c) 8 at% Cr, d) 12 at% Cr, d) 16 at% Cr.

effects of Cr concentrations on microstructural stability, thermal and mechanical properties. Figure 6.3 shows the phase stability of Cr containing alloys heat treated at 900°C for 168h. Additionally, Sauza (NU) investigated the mechanical properties and interfacial excess derived free energy for the Co-30Ni-7Al-4Ti-2W-3Mo-1Nb-1Ta alloy designed by **Lass** (NIST). It was shown that the alloy exhibits a high temperature yield strength exceeding that of commercial polycrystalline Ni-based superalloy MAR-M247. An atom-probe tomography study shows that Co partitions to the γ matrix, while Ni, Al, Ti, W, Nb, and Ta partition to γ' precipitates, and Mo segregates to grain boundaries, which results in an interfacial free energy reduction.

Coakley (NU) and **Lass** (NIST) compared creep induced rafting behavior in single-crystal multinary Co based alloy with a small W concentration (Co-30Ni-7Al-4Ti-2W-3Mo-1Nb-1Ta at%) and a Ni based superalloy (CMSX-4). It was demonstrated that under tensile creep, γ'-precipitates raft perpendicular to the applied load in Ni-based superalloys, whereas γ'-precipitates coarsen parallel to the applied load in our Co-based superalloy. Figure 6.4 shows the rafted microstructure for both Ni- and Co-based superalloys along different crystal planes. Furthermore, neutron diffraction measurements performed at Oak Ridge National Laboratory demonstrate that creep occurs predominantly in γ-channels in CMSX-4, whereas in the Co-based superalloy, both the γ- and γ'-phases deform during creep.

Co-Based CALPHAD Database Development A CALPHAD thermodynamic database has been constructed based on the Co-Al-W system through a collaboration between NIST, Wang (NU-NIST), Xiong (UPitt) and **Olson** (NU). Combined with the NIST Ni superalloy diffusion database, a preliminary elemental alloying design map is constructed for Co-based superalloys as shown in Figure 6.5. Slow diffusers with partitioning preferences to or phases can be identified to facilitate alloy microstructural design.

These thermodynamic and kinetic database successes have motivated **Olson** (NU) group design efforts to develop a new of Co-based superalloy that can be processed by additive manufacturing. Inconel 718 is considered as the benchmark alloy, setting the minimum requirements of the mechanical properties of the target alloy design. The present work

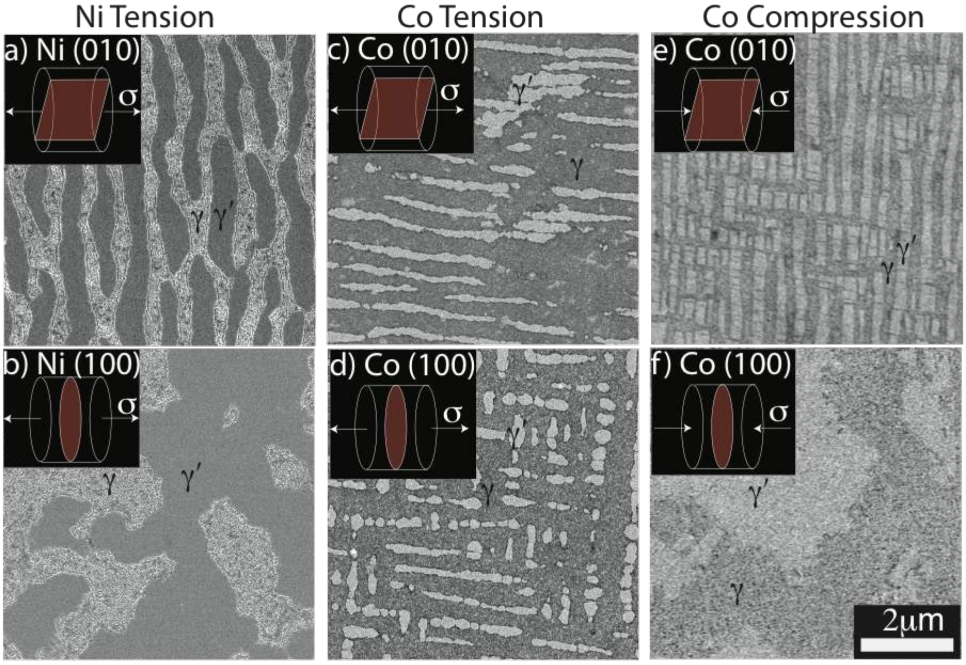


Figure 6.4: Secondary electron SEM micrographs of etched cross-sections displaying the γ-γ' rafted microstructure following creep of: a) (010) single crystal Ni-based superalloy crept in tension at 1150°C/100 MPa/10h; b) the corresponding (100) plane; c) (010) single crystal Co-based superalloy crept in tension at 940°C/100 MPa/20h; d) the corresponding (100) plane; e) (010) single crystal Co-based superalloy crept in compression at 940°C/100 MPa/20h; f) the corresponding (100) plane

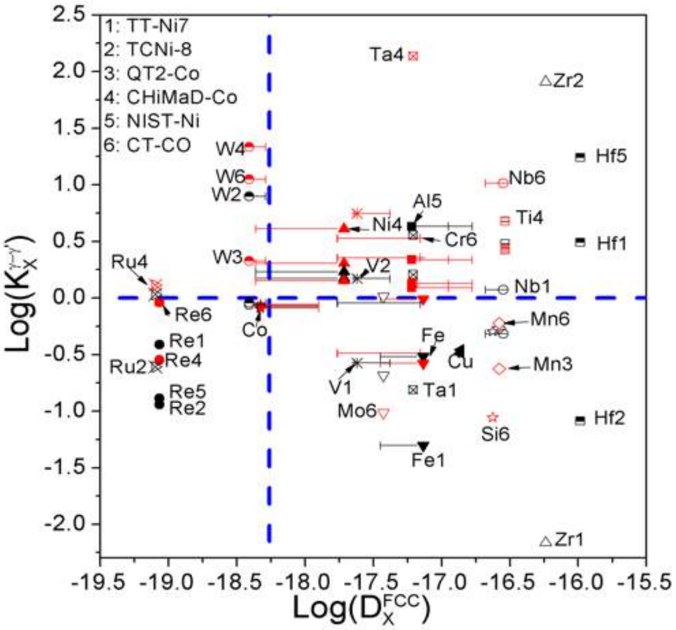


Figure 6.5: Map of elemental partition coefficient between γ and γ' and the diffusivity in matrix at 900°C. Red denotes Co-databases.

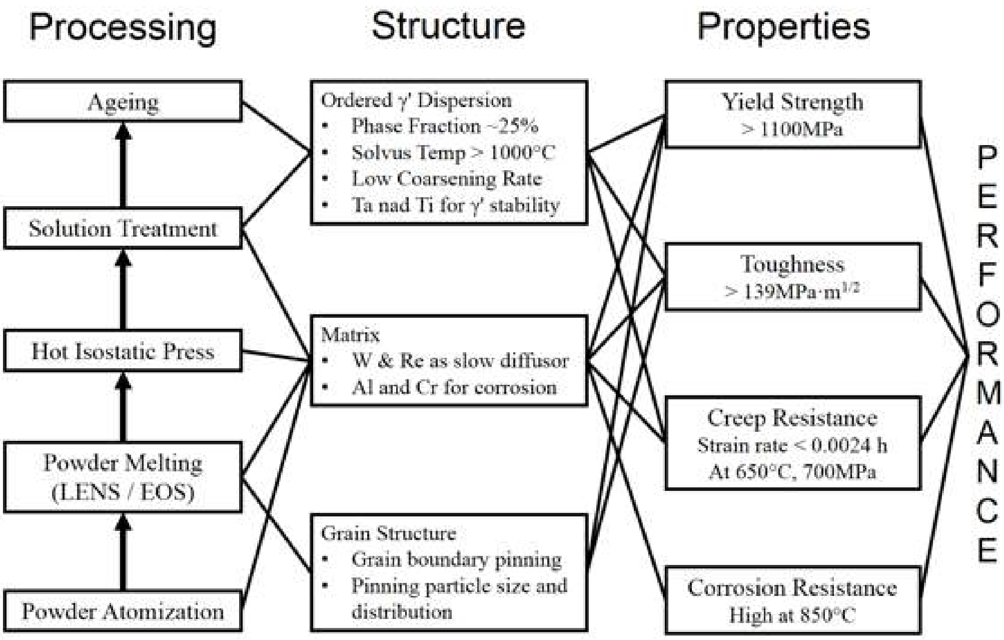


Figure 6.6: System design chart showing the process-structure-property relation for a Co-based superalloy designed for additive manufacturing

targets a Co-based candidate alloy with service temperature at 850°C, which is significantly higher than Inconel 718 (718°C). Primary design targets are tensile strength, toughness and creep resistance. Using the Systems Approach, strategies to produce these design targets can be identified by a system chart of the desired Co-based superalloy's process, structure, property relationships, shown in 6.6.

Based on the CALPHAD based ICME-modeling, the optimal design is an alloy with 22.93% γ' phase at 850°C with solvus temperature at 956°C. The model-predicted rupture time of this superalloy is 2555 hours higher than Inconel 718 (2411 hours). Figure 6.7 shows the elimination of detrimental phases occurring above 700°C. The predicted freezing range is about 97°C, which is suitable for additive manufacturing.

Olson (NU), **Campbell** (NIST), **Berardinis** (ASM), **Henry** (ASM) are engaging in an effort to develop a shared resource for CHiMaD Use-Case Groups to manage and analyze protodata stemming from their work. As a first step, the collaborators Dryer (Granta Design) and Searles (Granta Design) built a database using the commercially available Granta CES Selector and populated it with Co phase partitioning data transmitted in the form of XML files. The ability to import data in XML format is a critical requirement for the new resource based on the anticipated workflow associated with protodata. Provisions for running accelerated searches are also required, and one of the reasons for using CES Selector in the initial development stage. Through a series of demonstrations, ASM PIs demonstrated that the search tools on the CES platform could sort, filter, and plot the phase-based protodata, producing Ashby-type charts, as prototyped in Figure 6.5 and seen in Figure 6.8.

High-throughput Combinatorial Synthesis High-throughput experimental discovery efforts led by **Bedzyk** (NU) and **Chung** (NU) have extended previous high-throughput combinatorial synthesis procedures for Co-Ni-Ta and Co-Ti-Ta systems to include a vacuum annealing step prior to XRD experiments. This greatly reduces, and in some cases nearly

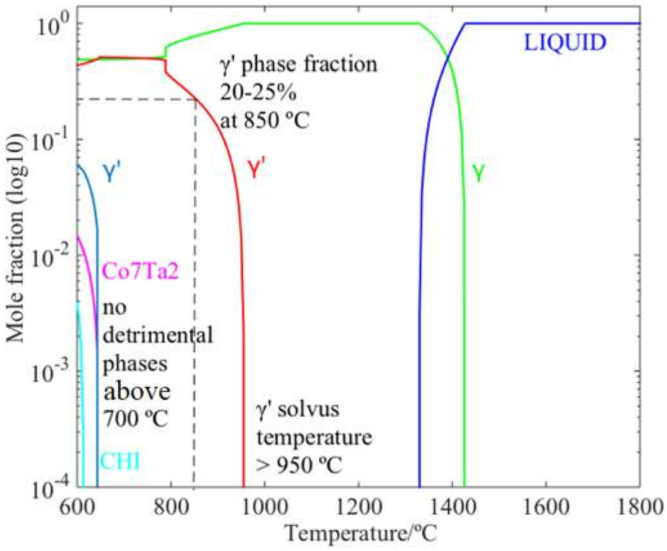


Figure 6.7: Step diagram of the designed Co-based superalloy

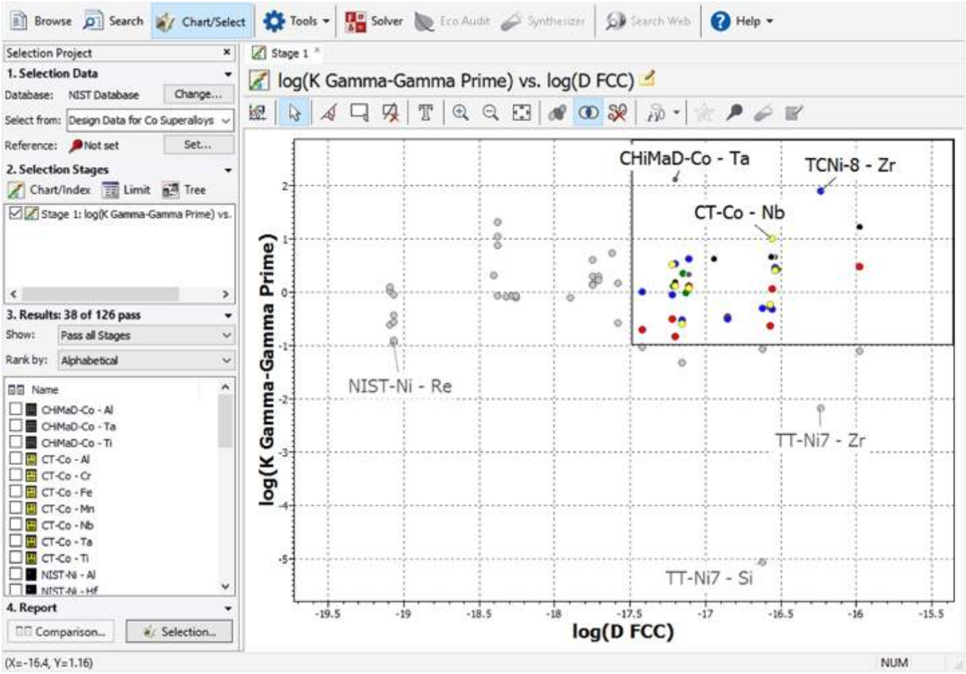

Selection Project
1. Selection Data
Database: NIST Database
Select from: Design Data for Co Superalloys
Reference: Not set
2. Selection Stages
☑ Stage 1: log(K Gamma-Gamma Prime) vs.
3. Results: 38 of 126 pass
Show: Pass all Stages
Rank by: Alphabetical
Name
☐ CHiMaD-Co - Al
☐ CHiMaD-Co - Ta
☐ CHiMaD-Co - Ti
☐ CT-Co - Al
☐ CT-Co - Cr
☐ CT-Co - Fe
☐ CT-Co - Mn
☐ CT-Co - Nb
☐ CT-Co - Ta
☐ CT-Co - Ti
☐ NIST-Ni - Al
☐ NIST-Ni - Hf
4. Report
(X=-16.4, Y=1.16)

Figure 6.8: A data plot generated by CES Selector can save users time by making data of interest more prominent and easier to find. Shown here are the results of a one-step graphical box selection of Cobalt phase data gathered by ChiMaD PIs

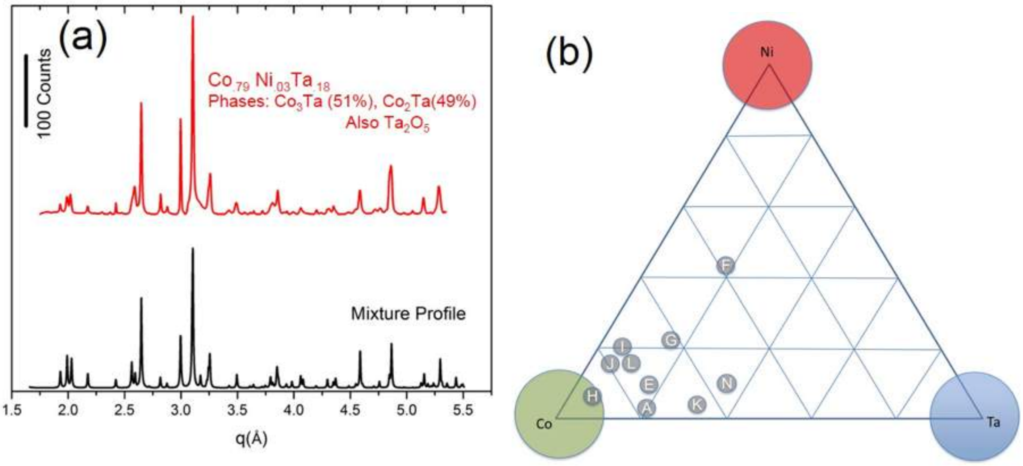


Figure 6.9: a) Mixture profile generated using *Crystaldiffract* based on phase information obtained from ICSD (black) and data from a sample of Co-Ni-Ta (red). The mixture profile contains Co_3Ta, Co_2Ta and Ta_2O_5. Corrections for preferred orientation and further refinement are not included, and b) composition mapping of Co-Ni-Ta sample wafers as measured by XRF. The phases observed for those compositions are listed in Table 6.1. All samples were annealed for 2 hours at 900°C prior to x-ray diffraction data acquisition at room temperature.

eliminates, the presence of oxides in samples. This is made possible through CHiMaD's funding of a high temperature vacuum furnace that can reach temperatures up to 1425°C at pressures below $3x10^{-6}$ Torr. Additionally, vacuum quartz encapsulation of samples with a water quench create isothermal slices of the phase diagram. Once a suite of analysis techniques for the XRD data is completed, a high-throughput roadmap will be developed for the study of other ternary systems.

Isothermal phase diagram representations have been successfully identified and synthesized containing many compositions with stable binary alloys of the Co-Ni-Ta systems, such as *hcp* Co_2Ta and rhombohedral Co_3Ta. The composition and phases observed show good agreement with available information from existing ASM databases. Progress on Co-Ti-Ta is carefully mapping previously unexplored ternary phase diagrams and identifying phases that are more prone to oxidation than the Co-Ni-Ta samples. Figure 6.9 shows a comparison between experimental data and a Co-Ni-Ta mixture profile generated using *Crystaldiffract* software based on phase information obtained from ICSD. The sample was annealed for 2 hours at 900°C prior to obtaining diffraction data.

New compositions are continued to be explored to discover previously undescribed binary and ternary phases. Further analysis of data from wafers quenched at temperatures between 550 - 900°C is expected to be fruitful. Integration of results with Thermo-Calc and DFT calculations are beginning to support and improve the results. The project continues to receive commendation for the experimental design from Argonne National Lab-Advanced Photon Source, where a majority of the characterization of wafers takes place.

DFT Calculations of Diffusion in Co and Interfacial energies Diffusion of various solutes in fcc-cobalt is poorly known, yet very important especially for processing and heat-treatment of superalloys. To address this problem, diffusion of various solutes in fcc-cobalt have been calculated using first-principles density functional theory (DFT), with these efforts led by Naghavi (NU) and **Wolverton** (NU). This demanding project has two main goals:

Sample	**Composition w/o O_2**	Phases (Rel. %) w/o Ta_2O_5
A	Co.79Ni.03Ta.18	Co_3Ta (46%) Co or Ni (54%)
E	Co.76Ni.10Ta.14	Co_3Ta (13%) Co or Ni (78%) $\gamma - Co_2Ta$ (9%)
F	Co.38Ni.44Ta.18	Co or Ni (70%) $Ta(CoNi_2)$ (30%)
G	Co.62Ni.22Ta.16	Co_3Ta (27%) Co or Ni (58%) $Co_{2.2}Ta_{0.8}$ (15%)
H	Co.90Ni.05Ta.05	Co or Ni(100%)
I	Co.74Ni.06Ta.20	Co_3Ta (35%) Co or Ni (50%) $Co_{2.2}Ta_{0.8}$(15%)
J	Co.77Ni.15Ta.08	Co or Ni(100%)
K	Co.64Ni.06Ta.30	$\gamma - Co_2Ta$ (100%)
L	Co.75Ni.10Ta.15	Co or Ni (91%) $Co_{2.2}Ta_{0.8}$(9%)
N	Co.54Ni.10Ta.36	Co_3Ta (51%) $\gamma - Co_2Ta$ (11%) $Ta(CoNi_2)$ (32%)

Table 6.1: Corresponding locations, composition, and wt% of phases excluding Ta_2O_5 for Figure 6.9b. Samples were annealed 2 hours at 900°C prior to testing at room temperature

i) to build a first-principles diffusion mobility database for fcc cobalt, and ii) to understand the key parameters that control the diffusion of a solute in fcc cobalt. This information is crucial to understand the macroscale properties of cobalt superalloys, such as diffusional phase transformations. Starting from self-diffusion in fcc cobalt, the effect of different exchange-correlation functionals on the vacancy formation energy, migration energy, and self-diffusion activation energy (Q) in fcc cobalt were considered. It was identified that Perdew-Burke-Ernzerhof (PBE) approximation has the best agreement with the available experimental data. A detailed analysis demonstrated that vibrational contributions are critical for an accurate calculation of self-diffusivity. To calculate diffusion coefficient of various solutes in fcc cobalt, DFT was used in conjunction with the five frequency model proposed by Lidiard and LeClaire. By this powerful combination, diffusion mobility of all 3d, 4d, and 5d transition metal (TM) elements, together with Al and Si have been calculated. Large solutes (20% larger than cobalt) have large diffusion coefficients due to a "strain-mediated mechanism." An approximation for the vibrational contribution to diffusivity for solutes was determined, which allows accurate values to be computed for the solute diffusivities at a reasonable computational cost. Extensive first-principles diffusion coefficients data for solutes in fcc cobalt will greatly accelerate the development and design of new cobalt-based superalloys.

As a part of collaboration with computational groups of **Heinonen** (ANL) and **Wolverton** (NU), and **Voorhees** (NU) along with experimental groups **Dunand** (NU), **Seidman** (NU), elastic constants of both γ and γ' phases at low and high temperatures were calculated. Interfacial energy and misfit strain of γ/γ' were also calculated for Co-based superalloys.

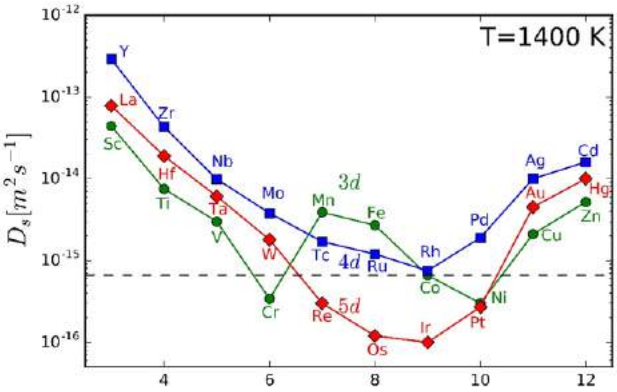


Figure 6.10: Relative Diffusivity of solutes in a Co-matrix at $T = 1400^\circ K$

This data serves as valuable, quantitative input to a predictive phase field model of the γ/γ' microstructural evolution in cobalt-based superalloys. A computational model has been developed for the prediction of the equilibrium shape of γ' inclusions in a γ-phase matrix of Co-W-Al alloys. The results are presently being written for submission to Acta Materialia.

High-Performance Shape Memory Alloys Liu (NU), supervised by **Olson** (NU), focused on the development of biocompatible, ultra-high cycle fatigue resistant PdTi-based Shape Memory Alloys (SMAs) for biomedical applications, including heart valve replacements and coronary stents. The system chart for the design of precipitation strengthened high-performance SMAs is shown in Figure 6.2. The coherent precipitation of nanoscale L21 Heusler aluminides has already been demonstrated to provide excellent strengthening and resistance to accommodation slip. Phase relations, precipitation kinetics, transformation temperature, transformation strain, cyclic stability, and mechanical properties were characterized in both Ni-free (Pd,Fe)(Ti,Al) and low-Ni high-strength hybrid (Pd,Ni)(Ti,Zr,Al) systems. Both DFT calculations and experimental data from Ni(Ti,Zr,Al) indicated that Zr is a promising addition to enhance Heusler precipitate shear modulus in the (Pd,Ni)(Ti,Al) system, resulting in a large modulus mismatch producing enhanced precipitation strengthening. These two designs, however, failed to provide higher strengthening than the previous quaternary (Pd,Ni)(Ti,Al) system. Misfit strains have been calculated of the hybrid alloy ($Pd_{30}Ni_{20}Ti_{38}Zr_8Al_4$) to be -0.02% after aging at 600°C, which is much lower than misfits computed for previous systems. Based on these calculations, a precipitation-strengthened PdTi-based SMA with higher misfit was designed in collaboration with a student team comprised of undergraduates and graduate students in Northwestern's Materials Design (MSE 390) class taught by Prof. Olson.

Fatigue Nucleation Modeling Continued collaboration between **Olson** (NU) and **Liu** (NU) involves fatigue nucleation modeling of SMAs and the effect of oxide inclusions. The ultra-high cycle fatigue life is governed by crack nucleation rather than growth in NiTi. Therefore, the control of non-metallic inclusions is of great importance due to their role as fatigue crack nucleants. Previous crystal plasticity finite element (CPFE) analysis modeling crack nucleation crystal plasticity examined the relationship between inclusion microstructure with fatigue life. This work explored the distance at which the free surface interacts with an inclusion and the effect of applied strain of surface-inclusion interaction.

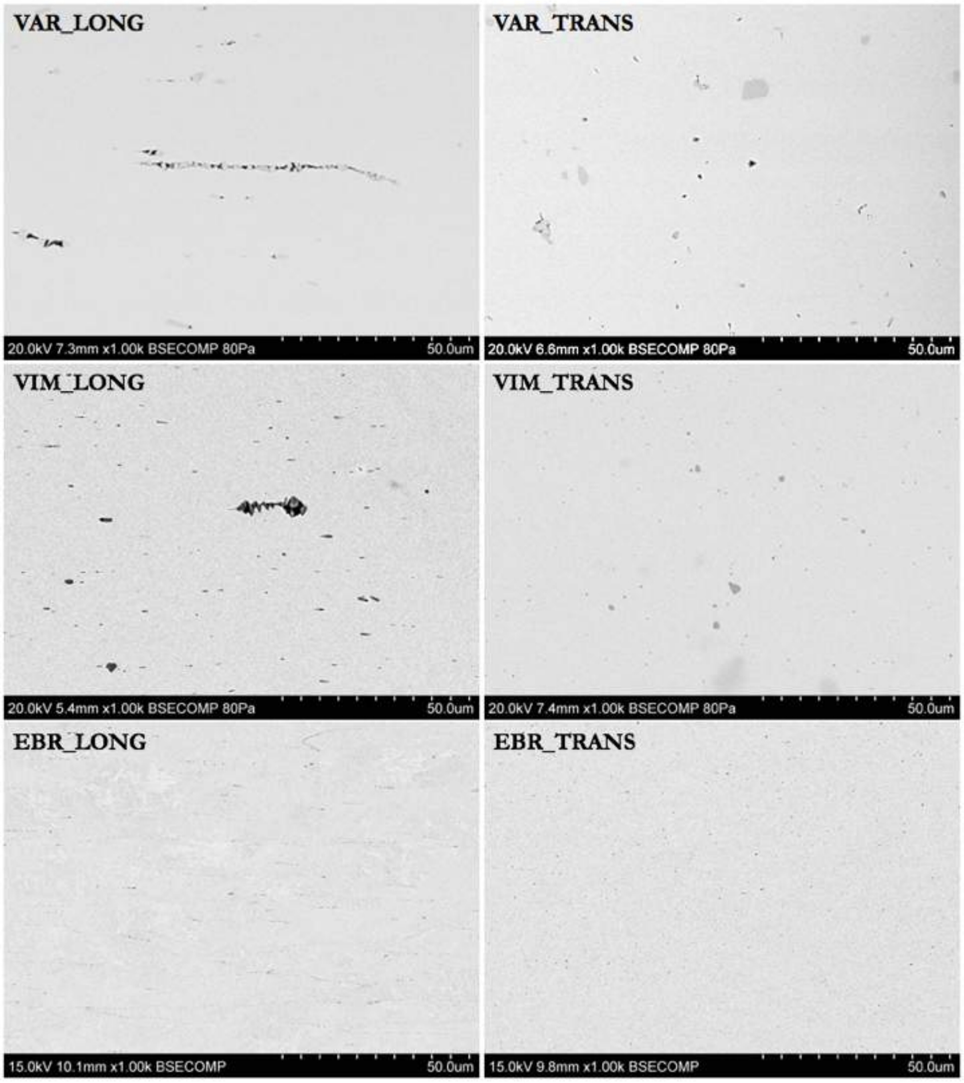


Figure 6.11: Representative backscatter electron micrograph of inclusion microstructure of NiTi tubes produced by vacuum arc remelting (VAR), vacuum induction melting (VIM), and electron beam refining (EBR).

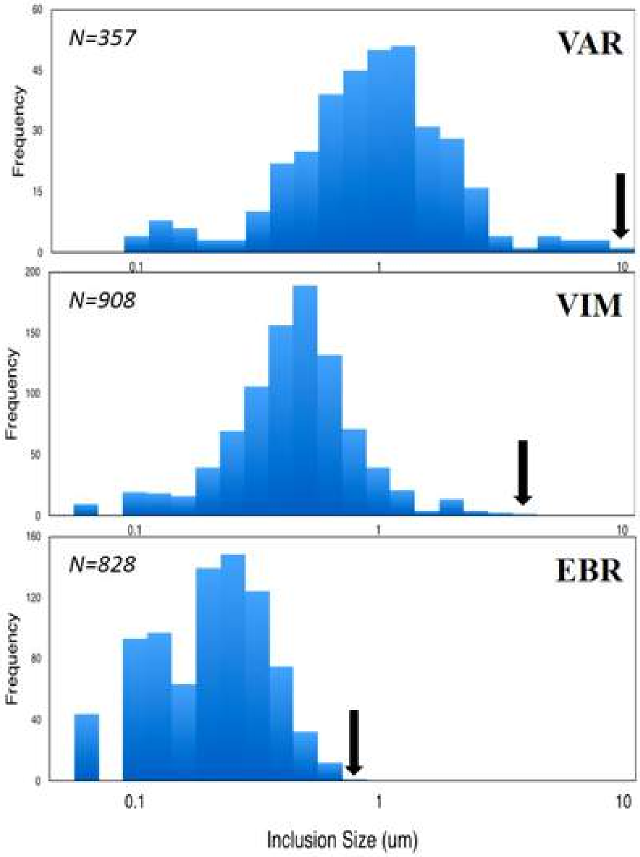


Figure 6.12: Process Optimization for Inclusion Refinement: Comparison of histograms of inclusion sizes (μm) produced in NiTi tubes in vacuum arc remelting (VAR), vacuum induction melting (VIM), and electron beam refining (EBR). EBR material indicates a smaller inclusion size, which indicates fatigue life may be improved when NiTi tubes are produced by this process.

It also investigated the effect of inclusion-inclusion interaction, inclusion size and matrix strengthening on fatigue life. The results indicated that process optimization to reduce voiding and debonding will increase fatigue performance, and stringers formed from fractured inclusions will be more detrimental than naturally occurring clusters of intact inclusions. It is, however, quite expensive to conduct CPFE analysis for a domain with defects cluster. An efficient fatigue prediction approach has been proposed, combining the reduced-order modeling technique named self-consistent clustering analysis (SCA) with CPFE. This approach has been identified in a J2 plasticity case to greatly reduce the computation time while keeping most of the local information needed for the calculation.

According to these modeling results, controlling inclusion size by processing routes is key to further improving the UHCF life. Three different processing routes have been studied to investigate their effect upon inclusion distributions in NiTi tubes (Figure 6.11). Due to the high internal pressure during cold drawing, non-metallic inclusion particles break up into long stringer clusters that act as potential crack nucleation sites. Stringers of length greater than $50\mu m$ can be found in a sample produced by vacuum arc remelting (VAR). On average, smaller stringers, about $20-30\mu m$, can be observed in a sample produced by vacuum induction melting (VIM). The third process of Electron Beam Refining (EBR), produces a sample in which most stringers are less than $10\mu m$ while the maximum is

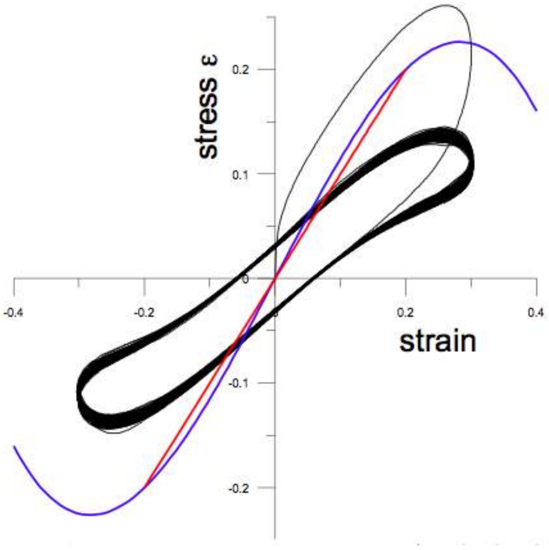


Figure 6.13: Dynamic stress-strain curve of cyclic loading

still about $20\mu m$. Of particular relevance to longitudinal fatigue properties controlling the life of medical devices is the transverse inclusion dimension. Ongoing quantification Liu (NU) is summarized in Figure 6.12, showing a substantial reduction in maximum particle size for the EBR materials. By these inclusion comparisons, it is predicted that the EBR processing may possess a better mean fatigue resistance than VIM. To achieve a significant increase in fatigue life, new processing method like spray forming may eliminate stringer formation during cold drawing.

During this period, the **Liu** (NU) group has advanced computational ability to create high-quality meshes for mechanical material simulations. This will produce higher accuracy simulations for fatigue prediction. Preliminary experiments have been conducted with the **Olson** (NU) group to generate the 3D input data required for these simulations. However, the most significant work is to couple crystal plasticity-based methods for fatigue prediction to a new reduced-order modeling framework developed by the **Liu** (NU) group. This will facilitate much more tractable simulation of large volumes and will enable the discovery of interactions occurring in large clusters (e.g. full stringers in NiTi or groups of voids in AM metals).

Phase field work by **Umantsev** (FSU) continues with Homogeneous Nucleation and LPSO Structure Formation models that were finalized and respective articles were published. Work has also begun regarding the application of Phase-Field modeling to ductile fatigue fracture. This model includes dynamic viscoplasticity and fracturing as a *phase transition* process. The model describes evolution of the viscoplastic medium including the work hardening and Baushinger effect (Figure 6.13).

Industrial Accelerated Qualification of Materials: Co-alloy Development QuesTek continues development of its previously designed Co-based aerospace bushing alloy (QT-Co) as a replacement for Cu-Be containing materials. Although QT-Co has been demonstrated to meet all primary property requirements in testing by Northrup Grumman, issues remained with meeting composition specifications (carbon specifically, being necessary to maintaining fine grain sizes through a grain refining TiC dispersion). During year two, these issues were addressed and QuesTek (**Sebastian**, **Snyder**, **Saal**, **Berglund**) successfully cast a

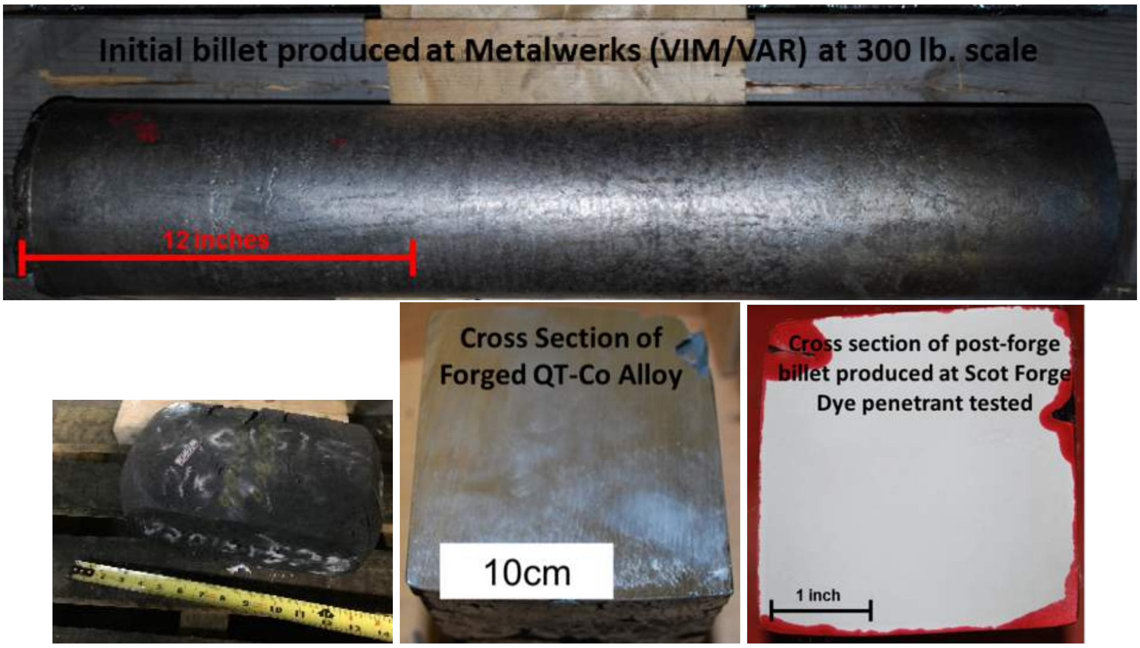


Figure 6.14: QT-Co alloy prior to forging (upper), post forging (lower left); cross-sectioned (middle); and (right) dye penetrant tested to ensure crack-free core

300-lb. heat of QT-Co with the target nominal composition, including carbon, produced by means of vacuum induction melting (VIM) followed by vacuum arc re-melting (VAR), according to the standard aerospace practice.

The year three effort has focused on applying optimized process conditions to convert the QT-Co ingot to convert to forged bar. A final product size of 3-inch (7.62cm) diameter has been selected to be relevant for common aerospace bushings. The material was delivered to *Scot Forge* (Spring Grove, IL) for homogenization and conversion to 3-inch diameter forged bar, however issues arose in forging due to surface cracking. The QT-Co material before and after forging is shown in Figure 6.14.

Following delivery of the forged material, QuesTek (**Berglund**, **Houser**, **Saal**, **Snyder**) undertook a full experimental assessment of solution and aging heat treatment response, to validate model predictions of optimal thermal processing. This included double-step aging trials as informed by *PrecipiCalc* simulations of accelerated precipitation response and enhanced tensile yield strength. A microstructural investigation of the as-forged core material showed primary particles identified by scanning electron microscopy energy dispersive spectroscopy (SEM-EDS) examination. The morphology elongated along the forging direction indicates these precipitates developed during forging. To investigate the source of cracking during forging, differential scanning calorimetry was utilized to validate the gamma prime solvus temperature, which showed the temperature was close to that of the thermodynamic prediction. A solution treatment study identified a final temperature of 1100°C for full solution. Aging study results are shown in Figure 6.15, which demonstrate a multi-step aging treatment of 800°C/30 hours + 680°C/4 hours provides equivalent hardness to the initial baseline of 780°C/72 hours.

In collaboration with an Air Force SBIR program at QuesTek, sub-scale bushing trials were also conducted to assess the wear and galling resistance of the forged alloy in the original (1-step aging) process condition. Post-test images of the QT-Co alloy bushings,

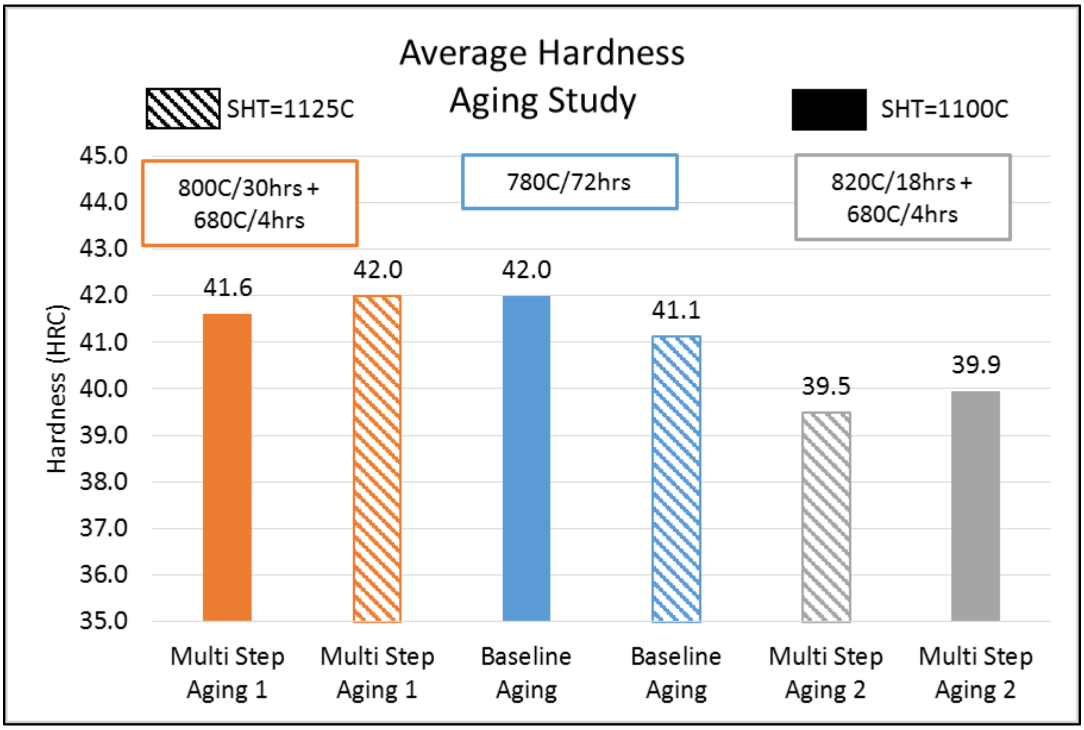


Figure 6.15: Aging study performed on QT-Co at various solution heat treatment times and aging treatments, which show similar hardness values for both the baseline aging treatment and the multi-step aging treatment 1 (HRC 41.5-42

test pins, and bushings in the test paddle are shown in Figure 6.16. The QT-Co bushings did not experience failure during testing, ran to the maximum load limit, and the test cycle ran slightly over the 2000 cycle standard for this test. The QT-Co alloy bushing test result is shown in Figure 6.17, along with the current Cu-Be alloys as well as the Toughmet Cu alloy. Overall, the results showed QT-Co meets the targeted value for maximum wear regardless of the type of evaluation (dimensional vs specific), and comparable to the incumbent Cu-Be.

The galling test was performed in accordance with ASTM G98. The setup is illustrated in Figure 18 along with the test results, which shows no galling was seen up to yielding in either QT-Co or Cu-Be. This confirms QT-Co has equivalent galling resistance to Cu-Be.

Figure 6.16: QT-Co alloy bushings after wear testing, showing low wear on both the bushing and the Cr-plated pin, indicating successful testing

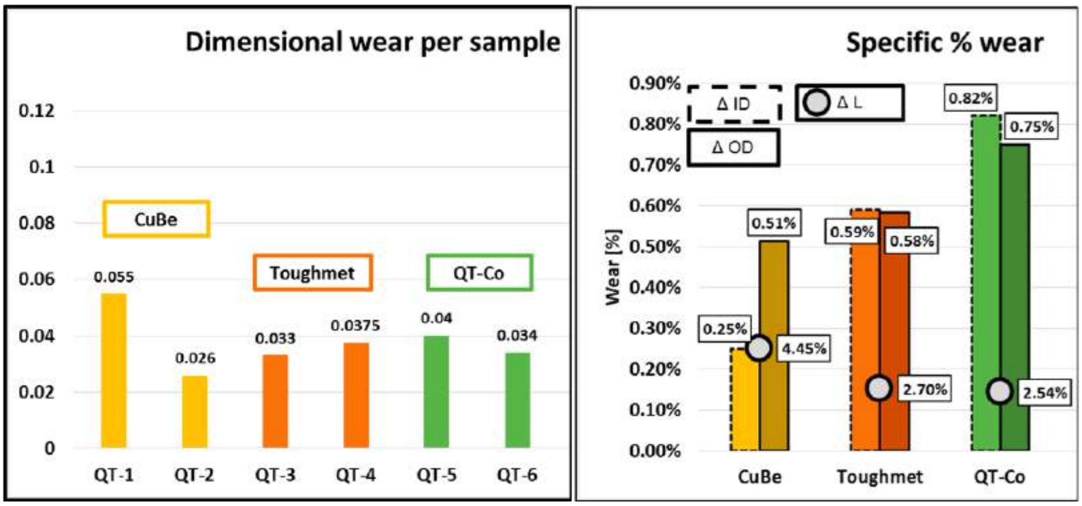


Figure 6.17: Left: Total dimensional wear of each bushing sample, color coded by alloy with the total wear shown in inches. Cuprium samples are indicated as *cracked* which corresponds to the post-test inspection. Right: Specific % wear for inner diameter (ΔID, dashed outline), outer diameter (ΔOD, solid outline), and length or thickness (ΔL, grey circle with black outline). All values correspond to the performing below the program diametric wear goal of less than 0.9% in both ID and OD change.

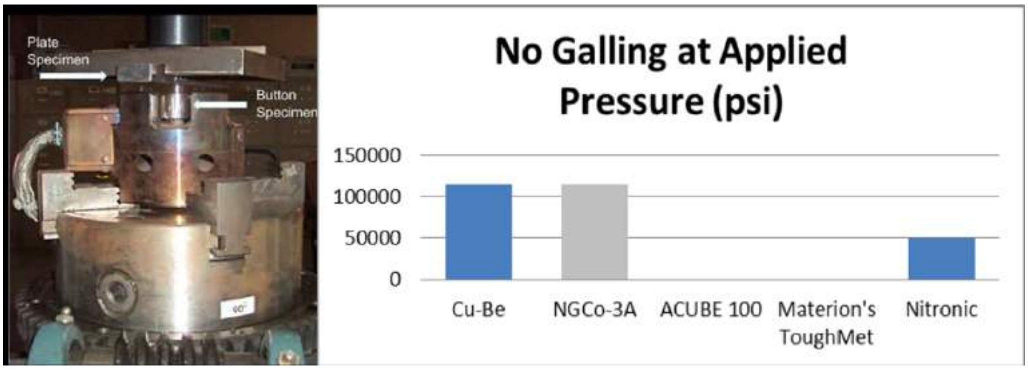


Figure 6.18: Photo of the galling resistance test setup (left), and *Northrop Grumman*-collected ASTM G98 galling test data (right), of QT-Co which shows similar results to Cu-Be in evaluation (i.e, no galling up through all tested stresses). ACUBE 100 and Toughmet (shown in this plot) were evaluated by *Northrop Grumman* in this initial test plan but were not selected for Galling evaluation

Industrial Accelerated Qualification of Materials: Shape Memory Alloy Development Year three efforts for QuesTek also focused on development of a medical material based on a patented PdNiTiAl nanoprecipitate strengthened shape memory alloy (SMA). This alloy is designed for superior cyclic stability, strength, fatigue resistance, biocompatibility and radiopacity compared to current NiTi SMAs. Internal activities at QuesTek, led by **Frankel** (QT), focused on improving these properties further through refinement of structure-property models and additional design iterations. Fatigue simulations modeling crack nucleation at non-metallic inclusions in commercial NiTi underscore the importance of increasing yield strength for ultrahigh cycle fatigue performance [25.54]. Controlled precipitation of nanoscale, low-misfit, L21 Heusler phase aluminides has demonstrated effective strengthening. Interphase misfit modeling at QuesTek, identified potentially improved strength by increasing the nanoprecipitate Heusler phase misfit with the matrix. To evaluate phase equilibria in the new quinary alloy, thermodynamic revision of QT-SMA database was performed. Informed by the precipitate misfit model and revised thermodynamic modeling, prototypes were designed, produced at the button scale, aging trials conducted, and the hardness response following aging tested. A National Institute of Health (NIH) Small Business Innovation Research (SBIR) proposal was submitted on the development of these Ni-free SMAs for biomedical applications in 2016.

Precipitation-Strengthened Thermoelectrics and CALPHAD development Work by **Voorhees** (NU) and Peters (NU), has been focused on building thermodynamic models and databases through the CALPHAD method to be used in optimizing Pb-based thermoelectric systems in collaboration with QuesTek and supported partially by the DARPA-SIMPLEX project. Thermoelectric materials could play a key role in meeting increasing global energy needs, but are currently limited due to their low efficiency. Current research is dedicated to investigating methods for improving their overall efficiency. One method is to introduce defects at various length scales that help scatter heat-carrying phonons thereby reducing the thermal conductivity of the material. Therefore, an ability to precisely control the microstructure of thermoelectric materials is fundamental in making them a viable energy solution. This has been done in numerous alloy systems and those tools can be applied here with similar success here. Similarly, nanoprecipitates can produce microstructural control of thermal conductivity if the system can be properly described by CALPHAD methods.

A five-sublattice model first developed by Chen et al for semiconductors has been used to model the binary PbX (X=S,Se,Te) systems. The model is unique to most other CALPHAD models as it contains explicit modeling for charge carriers. The carrier concentrations are used to fit parameters of the model, which are also supplemented with first-principle calculations for ionization and defect formation energies. A method for incorporating degeneracy into this model through the aid of first-principle calculations has also been implanted. Lastly, a two-sublattice model has been developed with common end-member descriptions that are compatible with multicomponent databases. These databases will be used in conjunction with a mobility database in order to optimize the thermoelectric properties in Pb based systems. This work was accepted and given an oral presentation at the XLV International CALPHAD Conference in Awajii, Japan.

Modeling efforts by **Stan** (ANL) regarding the development and computational framework predicting the change in thermal conductivity due to heterogeneous distributions of pores, design of thermoelectric materials progress towards microstructural design. Conversely, this method can determine the specific value of the pore shape factor corresponding to spe-

2016 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

  DMDII Rapid Qualification for Additive Manufacturing (Olson, Liu, Cao)
  -ICME AIM modeling of PH48S stainless maraging steel
  DARPA/Honeywell Open Manufacturing (QuesTek)
  - ICME for SLM additive manufacturing of Ni 718+
  DARPA-SIMPLEX: Data-Driven Discovery for Designed Thermoelectric Materials (QuesTek/CHiMaD)

CHiMaD

Figure 6.19: Steel Research Group (SRG) 2016 projects related to precipitation-strengthened alloys and design.

cific pore geometry. More importantly, the 3-D thermal transport framework can optimize the spatial distribution of porosity that maximizes or minimizes thermal conductivity. That can significantly improve the design of thermal conductors for power plant applications or thermal insulators for thermoelectric devices.

Steel Research Group (SRG) Projects and Design Class Interactions Northwestern University's SRG design consortium founded in 1985 now operates under CHiMaD auspices with the materials design research projects summarized in Figure 6.19. This notably includes the DARPA-SIMPLEX project integrating data analytics with microstructural design of thermoelectric materials. A new phase of the project has been organized where the experimental techniques for thin film combinatorics of metallic alloys developed by **Chung** (NU) and **Bedzyk** (NU) will be scaled up by *The Intermolecular* company to survey new intermetallic systems predicted by our data analytics.

The SRG and CHiMaD research projects provide a hierarchical project coaching system where graduate students serve as technical advisors to the class project teams summarized in Figure 6.20. Highlighted in red are projects supporting our new CHiMaD research directions of alloy designs constrained for 3D printing, including the Co alloy (Project V) described earlier in Figure 6.5 and Figure 6.6. The undergraduate team performing the Precipitation-hardened Austenitic steel design (Project II) place 2^{nd} in the ASM 2016 student design competition. All three 3dprinting alloy designs underwent preliminary experimental validation as arc-melted buttons Figure 6.20 by REU summer student Samuel Cabrera (UCI) working with Komai (NU). As-cast multiphase microstructures showed good agreement with predicted eutectic phases used to maintain hot cracking resistance.

MSc390 Materials Design
Spring 2016
Design Projects

I. **Q&P TRIP Steel**
Client: ArcelorMittal
Advisor: Amit Behera

II. **3D Printing Steel: PH Austenitic** ★
Client: NIST-CHiMaD, ONR, QuesTek
Advisor: Fuyao Yan

III. **HP Shape Memory Alloy (DTC)**
Client: NIST-CHiMaD, QuesTek
Advisor: Dr. Ricardo Komai, Paul Adler

IV. **HT Cast Aluminum**
Client: GM, DOE, QuesTek
Advisor: Andrew Bobel

V. **3D Printing Co Superalloy (ICME)**
Client: NIST-CHiMaD, QuesTek
Advisor: Dr. Wei Xiong

VI . **3D Printing TRIP Titanium**
Client: NIST-CHiMaD, DMDII, ONR, QuesTek
Advisor: Fan Meng

VII. **High ZT Thermoelectric**
Client: DARPA-SIMPLEX, NIST-CHiMaD, QuesTek
Advisor: Matt Peters

Figure 6.20: Design topics in the Northwestern University MSE 390 Materials Design course (**Olson** (NU)). The projects in red are those related to growing efforts in 3D printing and additive manufacturing. The project with the star (II), 3D Printing Steel: PH Austenitic was submitted to the 2016 ASM International student design competition and placed 2nd.

Printing Alloy Validation –S. Cabrera
(NSF-MRSEC REU; Advisor Dr. R. Komai)

- Co
- Steel
- Ti

Figure 6.21: Compositions designed from MSE 390 regarding a 3D printed Cobalt, Steel, and Titanium alloy were prototyped by CHiMaD REU student Samuel Cabrera (UCI). Alloy prototypes were then heat treated and examined for 3D printing feasibility.

6.4 Collaborations

6.4.1 CHiMaD Collaborations

Structural evolution of Co-based superalloys

*Christopher **Wolverton** (NU), Olle **Heinonen** (ANL)*

Wolverton (NU) group utilizes DFT to calculate some of the input parameters required by phase-field modeling performed by **Heinonen** (ANL) group.

Partitioning in γ/γ'

*Christopher **Wolverton** (NU), David **Dunand** (NU)*

Using DFT, **Wolverton** (NU) group will calculate partitioning in Co-based superalloys and compare the calculated results with available measurements performed by the **Dunand** (NU) group. This will allow for the interpretation of some peculiar trends observed in experiment and predict the partitioning of those alloys which to-date have not been measured by experiment.

Integrating CALPHAD and Data Mining for Advanced Steel Design

*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Gregory **Olson** (NU)*

This collaboration aims to use CALPHAD to enrich steel composition and processing data with structure information to derive more reliable data-driven structure-property linkages.

Steel fatigue data mining using processing and composition information

*Ankit **Agrawal** (NU), Alok **Choudhary** (NU)*

This project developed accurate forward predictive models for steel fatigue strength using a publicly available dataset, and also released an online software tool. Please see Section 12.5 for more information.

Thermoelectrics Data Mining

*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Gregory **Olson** (NU)*

This project aims at developing predictive models for thermoelectric properties of compounds and materials, and is primarily supported by the DARPA SIMPLEX project and managed by NAISE/CHiMaD.

Long-period Stacking Order Structure Formation

*Alexander **Umantsev** (FSU), Christopher **Wolverton** (NU)*

This collaboration focuses on the problem of calculating the free energy of a heterogeneous, two-phase structure using density-functional method.

Phase-Field Model of Ductile Fracturing

*Alexander **Umantsev** (FSU), Gregory **Olson** (NU)*

This collaboration focuses on phase field modeling of ductile fracturing and the comparison of the simulation results to experiments.

Modeling of Microstructural Evolution of Co-based Super Alloys

*Peter **Voorhees** (NU), David **Dunand** (NU), David **Seidman** (NU), Olle **Heinonen** (ANL), Christopher **Wolverton** (NU), Barry **Smith** (ANL)*

This collaboration focuses on complementing the efforts of the Precipitation Strengthened Alloys use-case group and utilizes phase field methods to determine the morphology of precipitates in Co alloys; a computational model for the equilibrium shape of γ' inclusions in a γ-phase matrix of Co-W-Al alloys. **Dunand** (NU), **Seidman** (NU), **Wolverton** (NU) groups provided the inputs such as interface structure, compositions, interfacial energies for the modeling lead by **Voorhees** (NU) and **Heinonen** (ANL) groups while **Smith** (ANL) was consulted for numerical and applied math issues that arose during the modeling.

Precipitation Strengthened Alloys

Peter ***Voorhees*** *(NU), Stephen* ***Davis*** *(NU)*

This collaboration focuses on developing models of rapid solidification of multicomponent alloys for use in additive manufacturing applications.

Lattice Misfit Measurement and Phase Identification using X-ray Diffraction

David ***Dunand*** *(NU), David* ***Seidman*** *(NU), Michael* ***Bedzyk*** *(NU)*

This collaboration utilizes x-ray diffraction to measure the lattice misfit between γ and γ' phases and to identify the crystal structure of other secondary precipitates.

Advanced Phase Field Methods

Marius ***Stan*** *(ANL), Olle* ***Heinonen*** *(ANL)*

This collaboration focuses on improving phase field models for predicting ionic transport in materials for energy storage applications (battery electrodes).

Uncertainty of Phase Diagrams

Marius ***Stan*** *(ANL), Peter* ***Voorhees*** *(NU), Gregory* ***Olson*** *(NU)*

This collaboration will focus on using multi-scale simulations and machine learning algorithms to evaluate the uncertainty of multi-component phase diagrams. In 2016, the directions of the research were discussed which will be implemented in 2017.

6.4.2 NIST Collaborations

Data-driven Design of Ni-Al-Cr Superalloy

Carelyn ***Campbell*** *(NIST), Shengyen* ***Li****, Ankit* ***Agrawal*** *(NU), Alok* ***Choudhary*** *(NU)*

This is a new collaboration that aims at using data-driven techniques to predict work-to-necking of a given Ni superalloy, and subsequently discover new superalloys with optimal desired properties.

Thermodynamic based Multinary Co Superalloys Design

David ***Dunand*** *(NU), David* ***Seidman*** *(NU), Eric Lass (NIST), Carelyn Campbell (NIST), Kil-Won Moon (NIST), Maureen Williams (NIST)*

Dunand (NU) and **Seidman** (NU) groups performed mechanical testing and microstructural characterization on multinary Co based superalloys designed by the NIST experimental group led by Lass (NIST). Iterative feedback based on characterization results aim to further improve the designed alloys. Graduate student Chung (NU) spent extended research time at NIST as a part of this collaboration.

Uncertainty of Phase Diagrams

Marius ***Stan*** *(ANL), Andrew* ***Dienstfrey*** *(NIST)*

This collaboration will focus on utilizing machine learning algorithms to evaluate the uncertainty of large thermodynamic data sets. In 2016, the directions of the research were discussed which will be implemented in 2017.

Uncertainty of Phase Diagrams

Marius ***Stan*** *(ANL), Ursula* ***Kattner*** *(NIST)*

This collaboration will focus on uncertainty of multi-component phase diagrams. In 2016, the directions of the research were discussed which will be implemented in 2017.

Co-Al-W-based Superalloys

Jason ***Sebastian*** *(QuesTek), James* ***Saal*** *(QuesTek), David* ***Snyder*** *(QuesTek), Ida* ***Berglund*** *(QuesTek), Dana* ***Frankel*** *(QuesTek), Clay* ***Houser*** *(QuesTek), Eric* ***Lass*** *(NIST), Carrie* ***Campbell*** *(NIST), Wei Xiong (UPitt), David* ***Dunand*** *(NU), David* ***Seidman*** *(NU)*

QuesTek has ongoing discussions with **Lass** (NIST), **Campbell** (NIST), and NIST-CHiMaD Postdoctoral Fellow Wang (NU-NIST), **Seidman** (NU), **Dunand** (NU), Xiong (UPitt) towards development of the Co-Al-W-based superalloys and related CALPHAD databases. QuesTek has provided literature reviews of relevant thermodynamic and kinetic data.

6.4.3 External Collaborations

Long-period Stacking Order Structure Formation

*Alexander **Umantsev** (FSU), Machiko Ode (NIMS, Japan)*

Formation of long-period stacking order (LPSO) lamellar structure observed in magnesium alloys is a novel example of precipitation strengthening mechanism in alloys. We developed a Ginzburg-Landau model of LPSO Structure Formation where, contrary to other models, LPSO is treated as a chemically modulated heterogeneous structure of parallel plates of two phases with different compositions and degrees of ordering. The results of this collaboration resulted in a publication in *Computational Materials Science* [25.59]

Synthesis of 3D printed Co-based superalloy foams for high temperature structural and functional applications

*David **Dunand** (NU), David **Seidman** (NU), Heeman Choe (Kookmin University, Korea)*

This collaboration focuses on synthesizing Co-Ni-W-Al-Ti quinternary Co superalloy through powder based 3D printing route follow by pack-cementation and heat treatment. Graduate student Park (Kookmin University) spent extended time at Northwestern University as a part of this collaboration.

Investigate the effect of Powder Metallurgy Approach in Co based Superalloys

*David **Dunand** (NU), David **Seidman** (NU), Monica Campos (University Carlos III de Madrid, Spain)*

This collaboration is developing and studying the effects of powder metallurgy processing approach in Co based superalloys. The goal is to develop new processing routes with advances cooling concepts to allow innovative designs for forming Co based superalloys. Graduate student Ferreras (University Carlos III de Madrid) spent extended time at Northwestern University as a part of this collaboration.

Machine Learning for Evaluating Point Defect Properties in Oxides

*Marius **Stan** (ANL), Bryce Meredig (Citrine Informatics)*

This collaboration will focus on the use of machine learning to evaluate thermodynamic properties of point defect and clusters in oxide materials, especially at high temperatures, and the impact on the uncertainty of oxide phase diagrams. In 2016, the directions of the research were discussed which will be implemented in 2017.

Air Force SBIR: AF151-160 Alternative Materials to Cu-Be for Landing gear Bushing/Bearing Applications

*Jason **Sebastian** (QuesTek), James **Saal** (QuesTek), David **Snyder** (QuesTek), Ida **Berglund** (QuesTek), Dana **Frankel** (QuesTek), Clay **Houser** (QuesTek)*

QuesTek was awarded this DoD SBIR under the Air Force to evaluate QT-Co as a replacement for Cu-Be in landing gear applications. Cuprium and Questalloy-Co were developed to replace the Cu-Be bushing alloys and offer similar mechanical properties, particularly equivalent or increased wear performance. In this program, QuesTek verified the mechanical properties of these alloys and demonstrated wear performance in representative coupon-scale bushing tests, comparing results to those of CuBE C17200 and other available alloy replacement candidates. (Contract #FA8222-15-M-0002)

NIH: Designed Shape Memory Alloy for SFA Applications

*Jason **Sebastian** (QuesTek), James **Saal** (QuesTek), David **Snyder** (QuesTek), Ida **Berglund** (QuesTek), Dana **Frankel** (QuesTek), Clay **Houser** (QuesTek)*

QuesTek has submitted a proposal to the NIH to validate a new superficial femoral artery stent material based on a patented PdNiTiAl nano-precipitate strengthened shape memory alloy (SMA) specifically designed for superior cyclic stability, strength, fatigue resistance, biocompatibility and radiopacity compared to current NiTi SMAs. In combination with recently developed novel processing, QuesTek's computationally-designed reduced-Ni SMA has potential to greatly enhance performance of cardiovascular, orthopedic, neural and other devices in medical applications that exploit superelastic (SE) material behaviors.

Galling Resistance Testing of QT-alloys *Jason **Sebastian** (QuesTek), James **Saal** (QuesTek), David **Snyder** (QuesTek), Ida **Berglund** (QuesTek), Dana **Frankel** (QuesTek), Clay **Houser** (QuesTek), Northrop Grumman Northrop Grumman* collected ASTM G98 galling test data for QT-Co which showed similar results to Cu-Be in evaluation (i.e, no galling up through all tested stresses). ACUBE 100 and Toughmet were evaluated by *Northrop Grumman* in their initial test plan but were not selected for Galling evaluation. Please see Figure 6.18.

6.5 Publications and Presentations

16 Number of CHiMaD-supported publications in 2016 by Precipitation-strengthened Alloys use-case group. Please see chapter 25 for details. [25.46, 25.47, 25.48, 25.49, 25.50, 25.51, 25.52, 25.53, 25.54, 25.55, 25.56, 25.57, 25.58, 25.59, 25.60, 25.61]

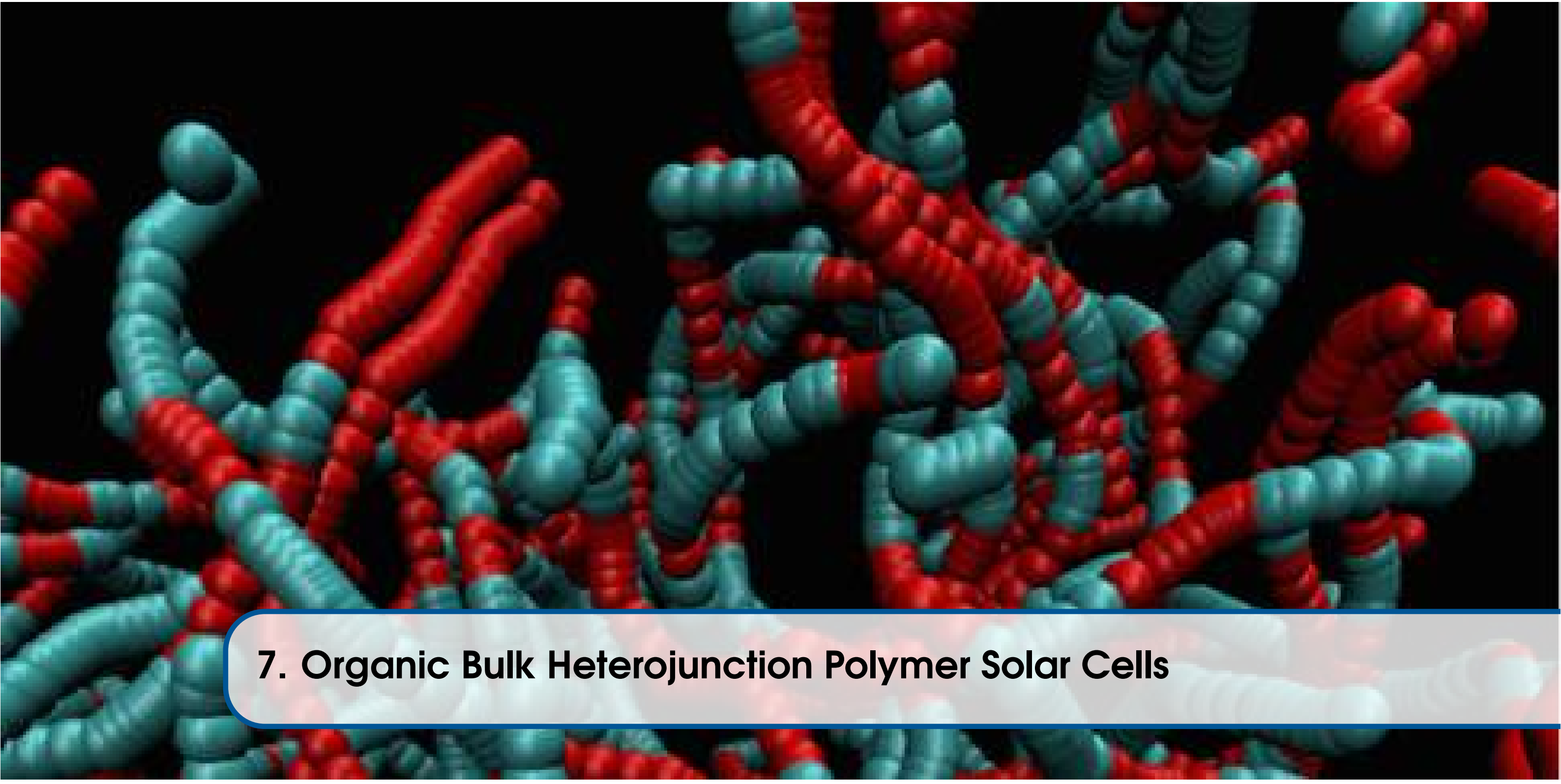
58 Number of presentations on CHiMaD supported research in 2016, please see section 24.13 for the complete list.

6.6 CHiMaD Team

Precipitation-Strengthened Alloys
Use-Case Group Researchers

Name	Position	Affiliation	Project (PI)
Gregory Olson	Principal Investigator	NU/MSE	
David Dunand	Principal Investigator	NU/MSE	
David Seidman	Principal Investigator	NU/MSE	
Wei Chen	Principal Investigator	NU/ME	
Christopher Wolverton	Principal Investigator	NU/MSE	
Ankit Agrawal	Principal Investigator	NU/EECS	
Alok Choudhary	Principal Investigator	NU/EECS	
Yip-Wah Chung	Principal Investigator	NU/MSE	
Michael Bedzyk	Principal Investigator	NU/MSE	
Wing Kam Liu	Principal Investigator	NU/ME	
Alexander Umantsev	Principal Investigator	FSU/PHY	
Jason Sebastian	Principal Investigator	QT	
David Snyder	Principal Investigator	QT	
James Saal	Principal Investigator	QT	
Ida Berglund	Principal Investigator	QT	
Dana Frankel	Principal Investigator	QT	
Peisheng Wang	Postdoctoral Researcher	NU/NIST	Co-Alloy database development *(Olson/Kattner/ Campbell/Lass)*
Wei Xiong	Research Associate	NU/MSE	Materials Design *(Olson)*
Zequn Wang	Postdoctoral Researcher	NU/ME	*(Chen)*
Shahab Naghavi	Postdoctoral Researcher	NU/MSE	DFT study of cobalt-based superalloys *(Wolverton)*
James A. Coakley	Postdoctoral Researcher	NU/MSE	Co-alloys *(Seidman/Dunand- EU Marie Curie Fellow - completed)*
Andrea Jokisaari	Postdoctoral Researcher	NU/NAISE	Modeling of microstructural evolution of Co-based super alloys *(Heinonen/Smith)*

Precipitation-Strengthened Alloys Use-Case Group Students			
Name	**Position**	**Affiliation**	**Project (PI)**
Daniel Sauza	Graduate Student	NU/MSE	Co-Alloys *(Dunand/Seidman- graduated)*
Qinyuan Liu	Graduate Student	NU/MSE	Fatigue *(Dunand/Seidman-Left CHiMaD program)*
Cameron Gross	Graduate Student	NU/MSE	High Throughput Combinatorial Synthesis and Analysis of Ternary Alloys *(Chung)*
Matthew Peters	Graduate Student	NU/MSE	CALPHAD Methods for Thermoelectrics *(Voorhees - NDSEG Fellowship)*
Logan Ward	Graduate Student	NU/MSE	Data Mining *(Wolverton-Graduated in 2016)*
Janak Thapa	Graduate Student	NU/MSE	High Throughput Combinatorial Synthesis and Analysis of Ternary Alloys *(Bedzyk)*
Chuan Liu	Graduate Student	NU/MSE	SMA for biomedical applications *(Olson)*
Cheng Yu	Graduate Student	NU/ME	Fatigue life prediction for advanced materials *(Liu)*
Orion Kafka	Graduate Student	NU/ME	Fatigue life prediction for advanced materials *(Liu-NSF Graduate Research Fellowship)*
Zheng Jia	Graduate Student	NU/ME	Mechanics of energetic materials *(Liu)*
Ding-Wen (Tony) Chung	Graduate Student	NU/MSE	Composition Design for Oxidation Resistance in Co-based Superalloys *(Dunand/Seidman)*
Francesca Long	Graduate Student	NU/MSE	Co-based Superalloys *(Dunand/Seidman)*
Furaha Ive	Undergraduate Student	FSU/PHY	Phase-Field Model of Ductile Fracturing *(Umantsev)*
Hyeji Park	Graduate Student (visiting)	NU/MSE	3D printed Co-based Superalloys *(Dunand/Seidman/ Shah/Choe(KU))*
Rafael Casas Ferreras	Graduate Student (visiting)	NU/MSE	Powder metallurgy processing of Co-based Superalloys *(Dunand/Seidman/ Campos(UC3M))*



7. Organic Bulk Heterojunction Polymer Solar Cells

Luping Yu (UC), Juan de Pablo (UC), Guilia Galli (UC), Tobin Marks (NU), Monica Olvera de la Cruz (NU)

Lee Richter Jr (NIST), Vivek Prabhu (NIST), Jack Douglas (NIST), Chad Snyder (NIST), Dean Delongchamp (NIST), Debra Audus (NIST), Kenneth Kroenlein (NIST)

Significance

Bulk heterojunction organic solar cells (OSCs) represent an alternative solar energy harvesting system, which is currently being pursued by numerous research groups world-wide. Commercial products are starting to appear in the market from several companies. This use-case group is addressing critical issues that affect the performance of OSC devices through materials design and synthesis to test new structure/function ideas, exploring new means of morphological control and its influence on OSC performance, new approaches to device optimization, data collection/analysis on new formulations and device characteristics, and on structure/property relationships. New electron donors or acceptors exhibiting superior photovoltaic properties are being developed, and their synergistic interactions are being studied. General rules for designing new polymers for use as charge relays or energy harvesting antennae in ternary OSCs are also being investigated. In close coupling to these experimental efforts, new theoretical methods are being developed to elucidate key electronic processes (electronic excitation, charge separation and transport) in our champion polymer systems and ternary polymer solar cells. To this end, large-scale modeling approaches are also being developed to simulate the morphology formation, polymer chain aggregation, and ways to control them. These studies are also closely coupled with efforts by NIST scientists to fully utilize their expertise in structural and morphological characterization of CHiMAD materials. These new materials and the basic knowledge gained will deepen our understanding of structure/property relationships and accelerate the development of OSCs towards more efficient and cost-effective commercial products.

7.1 Design Goals

The main design goal of the Organic Bulk Heterojunction Polymer Solar Cells use case group is to arrive at all-organic solar cells with reproducible efficiencies that are well above those of currently known for organic thiophene-based materials (ca. 8%). In the long term, a key aim of this group is to arrive at all-polymer organic photovoltaic materials that will obviate the need for fullerenes. The development of OPV materials to date has largely followed an Edisonian approach. This group seeks to identify key molecular and structural descriptors of performance which may be used in the future to rationally design improved materials for next generation OPV cells. To that end, the group is targeting the following activities:

- Develop novel ternary systems that can significantly enhance the power conversion efficiency (PCE) values of devices. Systematically survey the structures of third component polymers to establish structure/property relationship on energy level matching, template effects for self-assembly, and the relationship between composition and Voc values.
- Develop new types of polymers and small molecules with varied band gaps, energy levels, and optimized charge transport behaviors for use either as electron donors or acceptors in OSCs. Carry out detailed studies of structure property relationships.
- Develop efficient all-organic or all-inorganic, non-fullerene electron acceptors to replace fullerenes in OSCs.
- Develop new methods and force fields capable of fully describing aromatic semiconducting polymers.
- Model the electronic properties of these polymers based on sophisticated quantum mechanical calculations.
- Leverage NIST expertise by collaborating on several critical issues, including accurate measurement of glass transition temperatures, fullerene-polymer interaction, effect of new non-fullerene acceptors, and measurements of structure coupled to atomistic predictive simulations.

7.2 Significant Accomplishments in 2016

Ternary Blend Organic Solar Cells **Yu** (UC) group have developed a cluster type of electron acceptor, TPB, bearing four α-*perylenediimides* (PDIs), in which the four PDIs form a cross-like molecular conformation while still partially conjugated with the BDT-Th core. The blend TPB:PTB7-Th films shows favorable morphology and efficient charge dissociation. The inverted solar cells exhibited the highest PCE of 8.47% with the extraordinary high Jsc values ($> 18m/cm^2$), comparable with those of the corresponding PC71BM/PBT7-Th based solar cells.

Design of Building Blocks for Organic Semiconductor Materials **Marks** (NU) group made progress in design, synthesis and investigation of Sulfonamide Organic Photovoltaic Building Blocks. Conjugated small molecules and polymers based on the new π-*acceptor building block bithiophenesulfonamide* (BTSA) were synthesized. Molecular orbital computation, optical, electrochemical, and crystal structure analysis illuminate the architecture and electronic structure of the BTSA unit vs. other acceptor building blocks. Field-effect transistors and photovoltaic cells demonstrate that the BTSA is a promising unit for constructing π-conjugated semiconducting materials. **Marks** (NU) group also explored *diacetylenes* as Organic Photovoltaic Building Blocks. For the first time in the field of organic semiconducting/optoelectronic materials the incorporation and characterization of the *1,3-butadiyne* (*diacetylene*, $-C\equiv C-C\equiv C-$) moiety was achieved. Unoptimized OFET and OPV devices fabricated with the material demonstrate promising performance and excellent amenability to "morphological tuning".

Determination of Design Rules for New OPV Materials **Galli** (UC) group focused on establishing how the conformation of organic photovoltaic (OPV) polymers affects their electronic and transport properties, which is critical in order to determine design rules for new OPV materials and in particular to understand the performance enhancements recently reported for ternary blends. Coupled classical and ab initio molecular dynamics simulations showed that polymer linkage twisting significantly reduces optical absorption efficiency, as well as hole transport rates in donor polymers. It was predicted that blends with components favoring planar geometries contribute to the enhancement of the overall efficiency of ternary OPVs. Electronic structure calculations for the PTB7-PID2-PC71BM system showed that hole transfer rates are enhanced in ternary blends with respect to their binary counterpart. Finally, the results point at thermal disorder in the blend as a key reason responsible for device voltage losses and at the need to carry out electronic structure calculations at finite temperature to reliably compare with experiments.

Molecular Simulations of OPV-revelant Materials **De Pablo** (UC) group carried out molecular simulations of OPV-relevant materials and investigated the ring stacking behavior of single PTB7 molecules with and without its sidechains, and that of PTB7 in the bulk. It was found that single PTB7 molecules without sidechains show highly coiled configurations with an average 70% of the rings stacked for 50-mers, while steric hindrance in the full PTB7 molecule (with sidechains) reduces this value to 30%. Improved solvation in the bulk material of PTB7, as compared to PTB7 in the vacuum, increases end-to-end distance by a factor of 3 (for 50-mers) and increases stacking to 70%. New methods have also been developed by the **de Pablo** (UC) group to predict from atomistic simulations the chi parameters and Hansen solubility parameters for the polymers and solvents generally encountered in OPV formulations. In collaboration with the **Olvera de la Cruz** (NU) and **Richter** (NIST) groups, **de Pablo** (UC) also developed an extension of the TICG formalism for simulation of semi-flexible polymers and their blends. That formalism was used to predict the demixing of polymers encountered in OPV formulations.

7.3 Research Accomplishments

Development of Nonfullerene Acceptors The electron acceptors based on two ortho-position functionalized perylene diimide derivatives (αPPID, αPBDT) were synthesized as nonfullerene replacement in organic photovoltaic solar cells in **Yu** (UC) group. Due to the good planarity of ortho-position functionalized PDI and their enhanced intermolecular $\pi-\pi$ interaction, the αPPID and αPBDT show strong tendency to form aggregate. The packing order and domain structures are identical in blended film with PBT7-TH as in the pure film. The SCLC measurements showed high electron mobility. The inverted OPV cells based on αPDI- PBT7-TH exhibited the highest PCE of 4.92% for αPBDT based device and 3.61% for αPPID based device, which is 39% and 4% higher than that for their counterpart βPBDT and βPPID. The more efficient exciton dissociation at interfaces were observed between αPDI based compounds and PBT7-TH. The results suggest that α-substituted PDI derivatives are more promising electron acceptors for OPV than β-substituted ones.

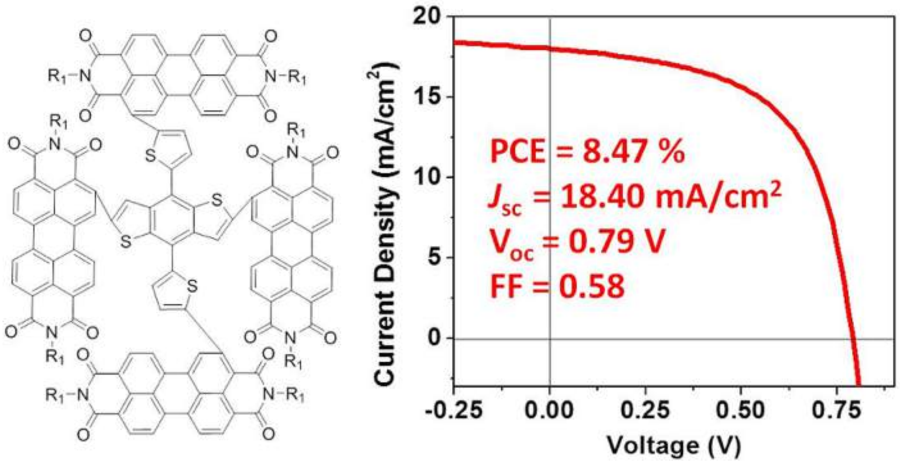


Figure 7.1: Molecular structures of αTPB and J-V curves of binary solar cells (PTB7-Th:αTPB).

Based on the work mentioned above, a significant development in the past year is synthesis and characterization of a cluster type of electron acceptor, TPB, bearing four α-perylenediimides (PDIs), Figure 7.1. The new electron acceptor contains four PDIs that form a cross-like molecular conformation while still partially conjugated with the BDT-Th core. The blend TPB:PTB7-Th films exhibit desired morphology and efficient charge dissociation. The inverted solar cells exhibited the highest PCE of 8.47% with the extraordinary high Jsc values ($> 18 mA/cm^2$), comparable with those of the corresponding PC71BM/PBT7-Th based solar cells. These materials were further evaluated by NIST scientists for deeper understanding in morphological effect.

OPV Materials Based on Bithiophenesulfonamide (BTSA) During 2016 the **Marks** (NU) group continued work on further developing OPV materials based on bithiophenesulfonamide (BTSA) - a conceptually new sulfonamide-centered building block designed and developed during CHiMaD years 1 and 2. Importantly, the inherent properties of sulfonamide group allow for efficient and scalable (gram-scale synthesis was easily demonstrated) preparation of the unit as well as materials based on it (Figures 7.2 and 7.3).

Another direction **Marks** (NU) group has been developing is the pioneering study and implementation of 1,3-butadiynes (diacetylenes) for organic semiconducting materials. The unique steric and electronic properties of the 1,3-butadiyne moeity include reduced steric bulk, a high degree of conformational flexibility, and a high density of accessible π-electrons. These properties suggest that this linkage may be an important tool for improving properties of semiconducting materials and offers opportunities for post-deposition functionalization.

Considering the importance of subunit dipole moment for the film morphology (crystalline domains, packing) and charge separation at donor/acceptor interfaces *[Chen, L. X., Yu, L., et al. J. Am. Chem. Soc., 2011, 133, 20468-20475]*, the BTSA building block was designed as unsymmetrical unit in order to obtain an increased dipole moment. Accordingly, donor-acceptor (D-A) polymeric materials involving BTSA can be obtained as regiorandom and regioregular polymers (Figure 7.2A). Importantly, it is known that for unsymmetrical subunits, the properties differences between regiorandom and regioregular polymers can be vast *[Wong, W. Y., Bazan, G. C. J. Am. Chem. Soc., 2011, 133, 18538-18541]*. Therefore we developed an efficient synthesis of regioregular BTSA-thiophene co-polymers (BTSA-

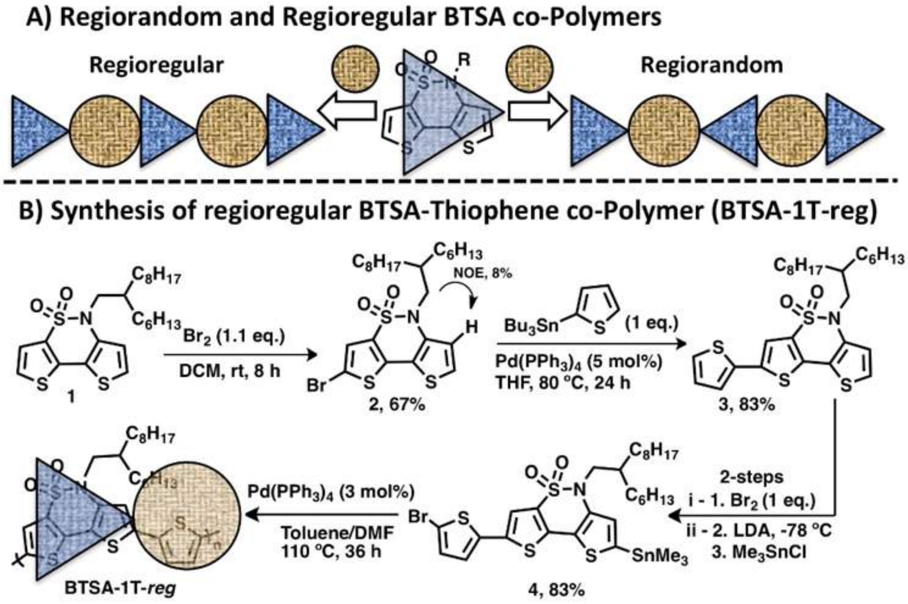
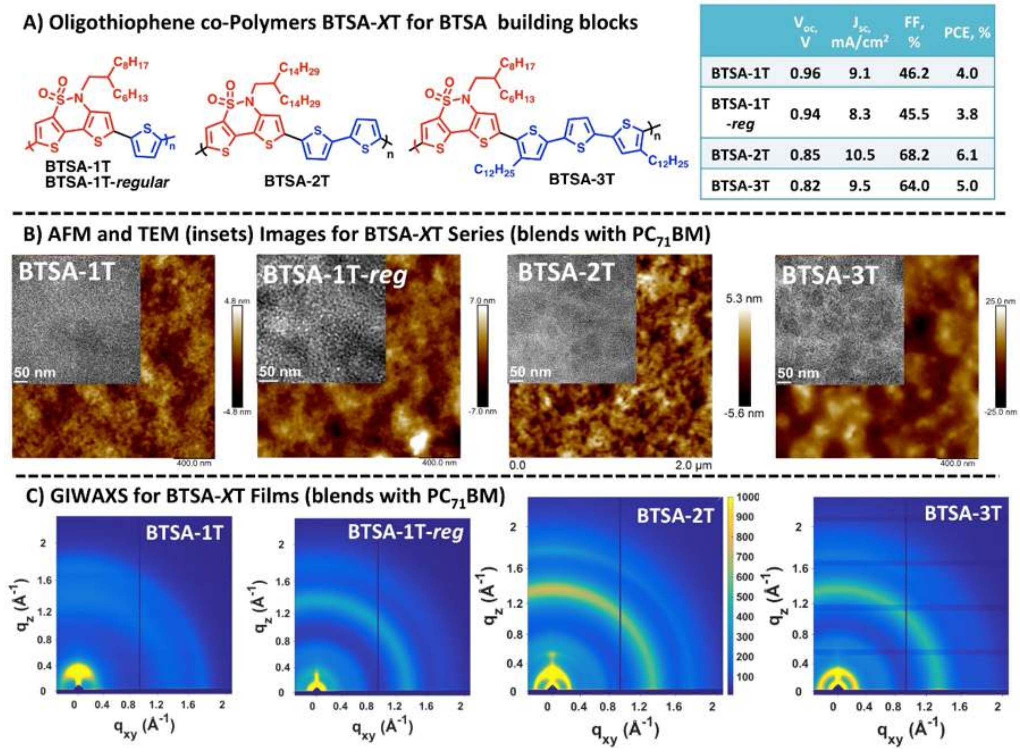


Figure 7.2: BTSA-based random and regular copolymers



	V_{oc}, V	J_{sc}, mA/cm^2	FF, %	PCE, %
BTSA-1T	0.96	9.1	46.2	4.0
BTSA-1T *-reg*	0.94	8.3	45.5	3.8
BTSA-2T	0.85	10.5	68.2	6.1
BTSA-3T	0.82	9.5	64.0	5.0

Figure 7.3: BTSA-*X*T co-polymers: A) Chemical structures and summary of BHJ OPV cell performance; B) AFM (height) and TEM images; C) GIWAXS diffraction images. All films were spin-coated using 5 mg/mL (polymer concentration) solution in CF:DCB (9:1) solvent mixture with 2% of DIO (1,8-diiodooctane) processing additive. Polymer:fullerene ($PC_{71}BM$) = 1:2 weight ratio was used.

1T-reg, Figure 7.3B) and compared its properties to regiorandom analogue. Next the photovoltaic performance and film morphology of a family of BTSA copolymers with oligothiophenes were studied in detail (Figure 7.3). Interestingly, BTSA-1T and BTSA-1T-*reg* exhibit almost identical photovoltaic performance with very high open circuit voltages (V_{oc}) and relatively low fill factors (FF). High V_{oc} is a result of the low-lying HOMO whereas low the FF likely results from the amorphous nature of the materials caused by the high volume of alkyl substituent chains, increasing the processability but compromising the tendency to form ordered domains. For BTSA-2T, the slightly lower V_{oc} (presumably resulting from the additional thiophene donor unit) and significantly higher FF (presumably resulting from the better crystallinity) compared to BTSA-1T materials is observed. Additional solubilizing chains were next placed on the flanking thiophenes to obtain solution-processable BTSA-3T copolymers. In spite of the significantly increased alkyl chain volume, which is usually detrimental to charge transport, and the extended *donor* unit where destabilization of the HOMO should be detrimental to V_{oc}, the BTSA-3T materials maintain a surprisingly high FF and V_{oc}. The relatively low short circuit current (J_{sc}) which limits the performance of the BTSA-3T based solar cells may be caused by the non-optimized molecular weights (M_n, M_w) and polydispersity (PDI) of the polymer. Further work is in progress in this regard. BTSA-XT/ PC71BM blend thin-film morphology was next studied with AFM, TEM, and GIWAXS techniques (Figures 7.3B, C). Surprisingly, both BTSA-1T regiorandom and regioregular materials form amorphous well-intermixed blends with fullerenes (AFM, TEM). As to the BTSA-2T and BTSA-3T materials, polymer/fullerene phase separation can be clearly observed in both AFM and TEM images. Interestingly, for BTSA-3T the fullerene clusters are better defined. Importantly, the size of the aggregates ($20-30nm$) is close to optimal as defined by the exciton diffusion length ($10nm$). Both BTSA-1T and BTSA-1T-*reg*. exhibit preferential *face-on* orientation of the polymer π-system relative to substrate plane. Interestingly, BTSA-2T neat films exhibit exclusively *edge-on*orientation, however the blends with fullerenes show predominantly isotropic organization. Preferential *face-on* orientation is also observed for the BTSA-3T-fullerene blend films. The most crystalline in the series are the BTSA-2T materials for both neat and fullerene blend films. The least crystalline is BTSA-1T, and no major differences are observed between regiorandom and regioregular materials. BTSA-3T crystallinity is in between of that of the 1T and 2T materials (Figure 7.3C).

Diacetylenes as Organic Photovoltaic Building Blocks Carbon-carbon triple bonds (alkyne motifs) has been used as an important tool for imparting a number of desired properties to organic semiconductors including stabilization of the frontier molecular orbitals (HOMO and LUMO), planarization of the conjugated backbone, reducing unfavorable steric interactions between in-chain π-blocks *[Facchetti, A., Marks, T. J., et al, Chem. Mater., 2012, 24, 2929-2942; Marrocchi, A., et al, Int. J. Mol. Sci., 2010, 11, 1471-1508]*. The more challenging and potentially more useful 1,3-butadiyne ($—C{\equiv}C—C{\equiv}C—$, diacetelene) moeity has never been explored in the field of organic semiconductors (Figure 7.4-1). To implement the 1,3-butadiyne motif in organic semiconductors we developed new alkyl-substituted 1,4-di(thiophen-2-yl)buta-1,3-diyne (R-DTB) donor building blocks, based on the $—C{\equiv}C—C{\equiv}C—$ conjugative pathway, and their incorporation with thienyl-diketopyrrolopyrrole (R'-TDPP) acceptor units into π-conjugated PTDPP-DTB polymers (P3, P4). The solubility of the new polymers strongly depends on the DTB and DPP solubilizing (R and R', respectively) substituents. Thus, solution processable and high molecular weight PDPP-DTB polymers are achieved for P3 (R = $n-C_{12}H_{25}$,

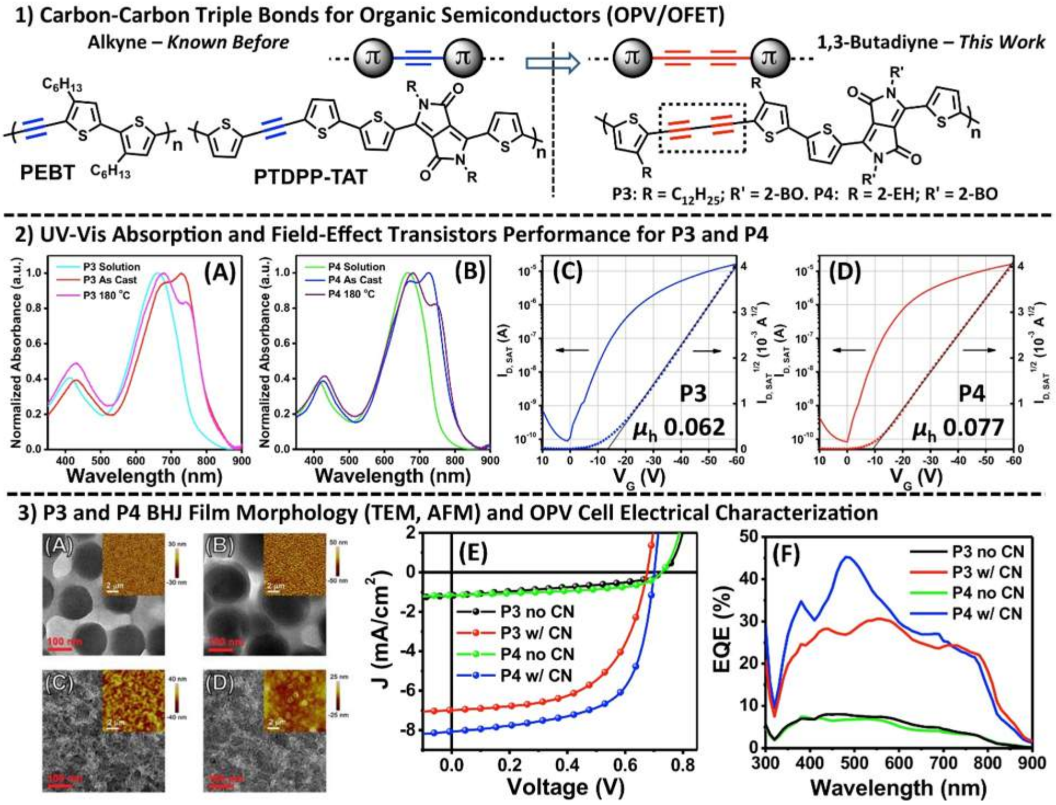


Figure 7.4: 1,3-Butadiyne-based building block for OFETs and BHJ OPV Cells. 1) Carbon-Carbon triple bond for organic semiconductors; 2) UV-Vis absorption spectra for P3 (A) and P4 (B); Bottom-Gate Top-Contact (BGTC) OFETs for P3 (A) and P4 (B); 3) TEM and AFM (inset) images for P3 and P4 blends with PC71BM processed without ((A), (B)) and with ((C), (D)) 1-chloronaphthalene (1-CN) additive respectively; (E) and (F) J-V characteristics and EQE spectra respectively. Films for device fabrication and morphology studies were spin-coated using 10 mg/mL (polymer concentration) solutions in $CHCl_3$: 1-CN (5% v/v) was added if necessary. Polymer:Fullerene ($PC_{71}BM$) = 1:2 weight ratio was used.

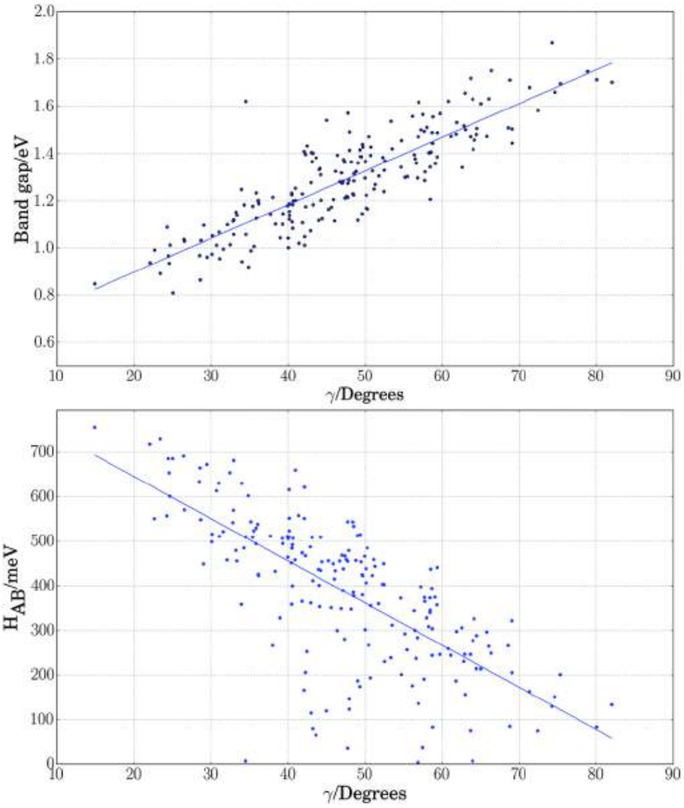


Figure 7.5: Band gap (computed at the PBE level of theory) and electronic coupling versus average non-planarity of PTB7 polymer chains

R'= 2-butyloctyl) and P4 (R = 2-ethylhexyl, R' = 2-butyloctyl). Systematic studies of P3 and P4 physicochemical properties were carried out using optical spectroscopy, cyclic voltammetry, and thermal analysis, revealing unique features of the dialkynyl motif (Figure 7.4-2). For the first time, optoelectronic devices (OFETs, OPVs) were fabricated with 1,3-butadiyne-containing organic semiconductors. OFET hole mobilities and OPV power conversion efficiencies approach $0.1cm^2/Vs$ and 4% respectively, which can be understood from detailed thin-film morphology and microstructural characterization using AFM, TEM (Figure 7.4-3). Importantly, DTB-based polymers P3 and P4 exhibit, in addition to stabilization of frontier molecular orbitals and to $—C{\equiv}C—C{\equiv}C—$ moderation of steric torsions, discrete morphological tunability through thermal annealing and processing additives. The advantageous materials properties and respectable device performance reported here demonstrate the promise of 1,3-butadiyne containing organic semiconducting materials.

Charge transport properties of semiconducting polymers in ternary OPV cells **Galli** (UC) and Goldey (UC) have examined the charge transport properties of polymers poly-3-oxothieno[3,4-d] isothiazole-1,1-dioxide/ benzodithiophene (PID2) and polythieno[3,4-b]-thiophene/benzodithiophene (PTB7) and the acceptor material [6,6]-phenyl C71 butyric acid methyl ester (PC71BM). Using electronic structure models, it was demonstrated that the twisting of conducting polymers increased the band gap and decreased critical along-chain hole conduction parameters for semiconducting polymers, as shown in Figure 7.5. This study was enabled by a collaboration with Reid (UC) from the **de Pablo** research group, whose molecular dynamics configurations were used for these calculations.

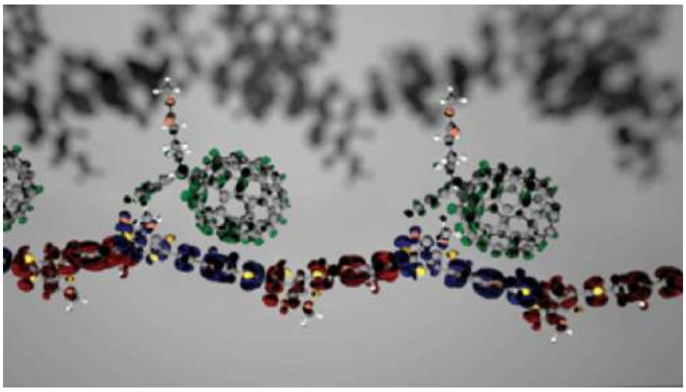


Figure 7.6: Model of PTB7 and PC71BM interface, showing isosurfaces of positive charge carriers

Using models of interfaces (shown in Figure 7.6), hole transfer rates was computed to evaluate the hypothesis of *[Lu, et al Nat. Photonics, 2014, 8, 716]* that PID2 facilitates more efficient hole extraction in ternary blends. We calculated hole transfer rates between different components, finding that holes transfer from PC71BM to PID2 6-8 orders of magnitude faster than those to PTB7. The slow hole transfer rates at the PTB7:PC71BM interface are due to the presence of a Marcus inverted region, where the driving force for hole transfer is sufficiently large that it increases the activation energy for that process. The calculated Marcus rates for hole transfers between PC71BM and PTB7 7.1 and PID2 is presented in 7.2. The results support the experimental observations.

Hole Transfer	$\Delta G(eV)$	k^{Marcus}, s^{-1}
PTB7-1 → PTB7-2	-0.07	$3.9 \times 10^{+15}$
PTB7-1 → PC71BM	0.76	1.3×10^{-2}
PTB7-2 → PC71BM	0.82	1.3×10^{-4}
PTB7-2 → PTB7-1	0.07	$3.0 \times 10^{+14}$
PC71BM → PTB7-1	-0.76	$8.8 \times 10^{+8}$
PC71BM → PTB7-2	-0.82	$4.4 \times 10^{+7}$

Table 7.1: Driving forces (ΔG, eV) and Marcus hole transfer rates (k^{Marcus}, s^{-1}) at the PTB7:PC71BM interface between two PTB7 subunits (denoted -1 and -2) and PC71BM

Hole Transfer	$\Delta G(eV)$	k^{Marcus}, s^{-1}
PID2-1 → PID2-2	0.14	$3.4 \times 10^{+13}$
PID2-1 → PC71BM	0.61	$3.2 \times 10^{+2}$
PID2-2 → PC71BM	0.47	$1.8 \times 10^{+6}$
PID2-2 → PID2-1	-0.14	$8.1 \times 10^{+15}$
PC71BM → PID2-1	-0.61	$3.8 \times 10^{+11}$
PC71BM → PID2-2	-0.47	$3.7 \times 10^{+13}$

Table 7.2: Driving forces (ΔG, eV) and Marcus hole transfer rates (k^{Marcus}, s^{-1}) at the PID2:PC71BM interface between two PID2 subunits (denoted -1 and -2) and PC71BM

Atomistic Simulation of the Champion Conjugated Polymer, PTB7, Chain Structures
De Pablo (UC) and Reid (UC) focused their research effort primarily on the atomistic simulation of the champion conjugated polymer, PTB7, identifying the mechanism of

power conversion efficiency enhancement in ternary OPV cells, as well as the application of free-energy sampling methods to understanding the solvent and additive-dependence of PTB7 solution-phase conformations.

Recently published work combining classical and ab-initio molecular simulation has demonstrated that increased planarity in PTB7 significantly enhances its optical absorption efficiency and hole transfer rates.1 Results show that the highly planar PID2 acts as a template for PTB7, increasing the degree of PTB7 planarity and thus improving electronic properties of the device. This newly-uncovered mechanism can be further exploited to tune planarity and efficiency within OPV systems.

Controlling the morphology of solution-processed OPV devices is a challenging task. To better understand solution-cast PTB7-PCBM morphologies we have utilized custom OPLS-based atomistic force-fields and applied free-energy sampling methods in a variety of explicit solvent environments to quantitatively predict the free-energy surfaces of conjugated polymer folding in the solution-phase. Simulations reveal that the common, but poorly understood, additive DIO swells PTB7 into a less-ordered state in solution - a result which is corroborated by optical measurements of polymer absorption in solution. These simulations also quantify fundamental design rules for solution-phase morphologies, such as the molecular weight dependence of the folding free-energy surface, and the influence of solvent mixtures on conjugated polymer conformations. Current efforts are focused on arriving at a framework for systematic prediction of Chi parameters and Hansen solubility parameters of OPV materials in relevant solvents.

An additional direction pursued in the **de Pablo** (UC) and **Olvera de la Cruz** (NU) groups has sought to extend the TICG models used in the DSA Use case to encompass the semi-flexible polymeric materials of interest to OPV applications. That effort has led to a powerful new model which has been shown to predict the demixing of rigi and flexible polymeric materials as a function of rigidity, concentration, and temperature.

'χDB' Database. The 'χDB' database has been led by **de Pablo** (UC) in collaboration with **Audus** (NIST) and **Foster** (UC/ANL) to implement a hybrid human-computer system that extracts Flory-Huggins parameters from the scientific literature. This approach is based on an ambitious attempt to create a digital handbook using automatic extraction and crowdsourcing. This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB project also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Figure 7.7 illustrates the number of polymer-polymer χ values in the database. Preliminary expert assessment showed that the literature-extraction approach is a promising strategy for the χ parameter. The χ DB digital handbook, populated by educating students in polymer science and engineering, is now available for material scientists to use and evaluate at http://pppdb.uchicago.edu/. it is currently being expanded to include other properties of polymers, beyond the χ parameter.

Application of machine learning algorithms have been prevailing in the development of "χ-DB". Using publications marked as 'relevant' and a machine learning software, "χ-DB" database has improved the publication selection process by decreasing the number of reviewed publications that do not contribute to the χ database from 60% to 14%. Participation of trained undergraduate students in the curation process has been proven

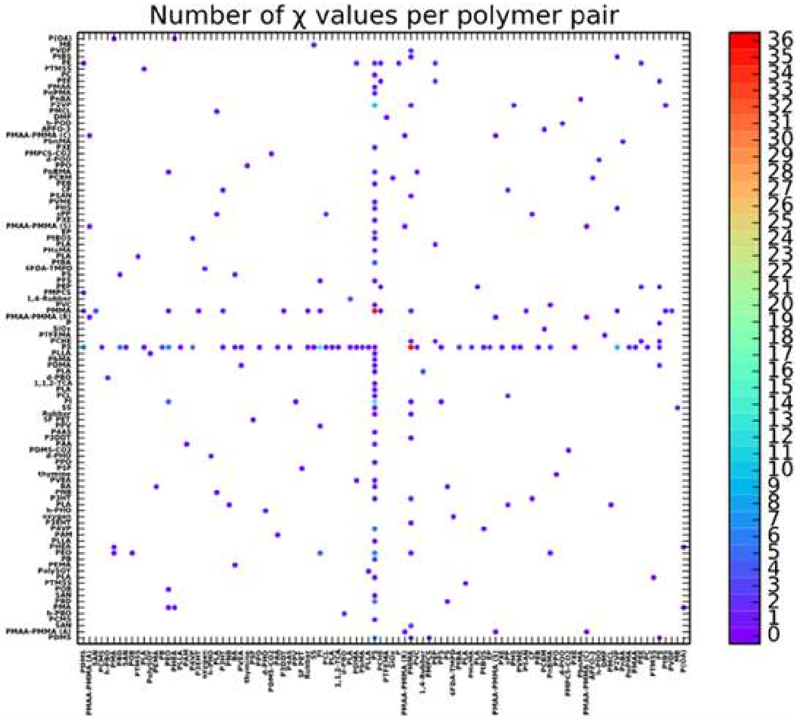


Figure 7.7: Number of χ values per polymer pair

effective in accelerating the data population progress and providing context for ontology development for "χ-DB". Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4].

7.4 Collaborations

7.4.1 CHiMaD Collaborations

Wide Band Gap Polymers

Luping ***Yu*** *(UC), Tobin* ***Marks*** *(NU)*

Yu (UC) group collaborated with **Marks** (NU) group on conducting morphological studies on wide bandgap polymer systems.

Simulations of on Ternary Blend OPV

Luping ***Yu*** *(UC), Guillia* ***Galli*** *(UC), Juan* ***de Pablo*** *(UC)*

This collaboration focuses on building a theoretical understanding of ternary OPV systems and electron acceptors.

Structure-property Relationships in Molecular Acceptors

Guillia ***Galli*** *(UC), Juan* ***de Pablo*** *(UC), Luping* ***Yu*** *(UC)*

This collaboration investigates the structure and properties of semiconducting organic molecules composed of perylene diimide dyes, which **Yu** (UC) group has been developing as optically-active photovoltaic acceptor materials. The researchers are investigating different connectivity motifs, as well as morphology in the condensed phase.

Structure-property Relationships in Ternary Blend OPV

Guillia ***Galli*** *(UC), Juan* ***de Pablo*** *(UC)*

Through this collaboration, models of semiconducting polymers for organic photovoltaics were generated. This has resulted in confirmation of an experimental hypothesis for why ternary blends outperform binary mixtures of photovoltaic materials.

Coarse Grain Modeling of All-Polymer Solar Cell Materials

*Monica **Olvera de la Cruz** (NU), Tobin **Marks** (NU), Juan **de Pablo** (UC)*

This collaboration focuses on modeling of donor polymer-acceptor polymer blends to understand molecular mass effects on blend rheology, mixing, microstructure, and photovoltaic response.

X-ray Scattering of Photoactive Organic Thin Films

*Michael **Bedzyk** (NU), Tobin **Marks** (NU)*

This collaboration focuses on the analysis of structural order in bulk-heterojunction organic photovoltaic materials using x-ray scattering techniques.

Microstructure Analysis of Bulk Heterojunction Photovoltaic Blends

*Vinyanak Dravid (NU), Tobin **Marks** (NU)*

This collaboration focuses on the analysis of phase separation, microstructure, and local atomic composition in bulk heterojunction photovoltaic blends by advanced electron microscopy techniques.

MD force field generation for Organic Bulk Heterojunction Polymer Solar Cells

*Guilia **Galli** (UC), Juan **de Pablo** (UC)*

The collaboration between **Galli** and **de Pablo** groups has focused on the generation and validation of an atomistic force field for simulations of the donor polymer PTB7. Several potential energy surfaces for calibration of internal coordinate parameters were calculated. **Galli** group has also used trajectories with this force field to statistically sample geometries for their electronic structure calculations.

7.4.2 NIST Collaborations

Morphological Measurements

*Luping **Yu** (UC), Lee **Richter** (NIST)*

This collaboration involved the measurement of morphology and OPV with nonfullerene acceptor, UPS for determining HOMO/LUMO energy level and the origin of V_{oc}/composition correlation in ternary solar cells. **Yu** group has synthesized deuteraed PTB1 polymer for solid state NMR studies by Richter (NIST) group. As a part of this collaboration, two graduate students Zhao (UC) and Shaparov (UC) has spent extended research time at NIST in Summer 2016. A publication on this collaboration is in preparation.

Thermal Analysis of All-Polymer Solar Cell Materials

*Tobin **Marks** (NU), Chad **Snyder** (NIST)*

This collaboration Investigates of the thermal properties of donor polymer-acceptor polymer blends to understand molecular mass effects on blend rheology, mixing, microstructure, and ultimately photovoltaic response.

χ-DB Database

*Debra **Audus** (NIST), Ian **Foster**, Juan **de Pablo** (UC), Matthew **Tirrell** (UC), Kenneth **Kroenlein** (NIST)*

Members of CHiMaD and NIST collaborate on development of automated tools for data extraction from the literature and creation of a data base of polymer properties for design of DSA processes. Audus (NIST) spent a month at the University of Chicago in 2015 participating in this collaboration and developing a course on data base creation. As part of this collaboration, a polymer property predictor tool was developed that includes models for homopolymers, copolymers, and charged polymers. Tchoua (UC) visited Kroenlein (NIST) at Boulder to discuss their efforts to extract literature data in the context of thermodynamic fluid properties for process design. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

7.4.3 External Collaborations

GWIXS of Ternary OPV Systems

*Luping **Yu** (UC), Wei Chen (Argonne National Laboratory)*

This collaboration with Chen group at ANL involves the experimental efforts regrading Grazing incidence wide-angle X-ray scattering (GWIXS) measurements of OPV systems this use-case is working on.

Ultrafast Spectroscopy

*Luping **Yu** (UC), Lin Chen (Argonne National Laboratory/ Northwestern University)*

This collaboration with Chen group at ANL involves the experimental efforts regrading ultrafast spectroscopy measurements of OPV systems this use-case is working on.

Sulfonamide Organic Photovoltaic Building Blocks

*Tobin **Marks** (NU), Antonio Facchetti (Polyera Corporation)*

This collaboration focuses on the fabrication of field-effect transistors using industrially related, compatible with printing technologies solution processable dielectric materials (CYTOP, PMMA) for study the charge transporting properties of sulfonamide-based materials as well as testing of OPV cells using sulfonamide-based are performed in collaboration with *Polyera* Corporation.

7.5 Technology Transfer

Patent

Bithiophene Sulfonamide-Based Molecular and Polymeric Semiconductors

A. Facchetti, T. J. Marks, Y. Xia, M. Drees, F. Melkonyan, W. Zhao

Date: May 26, 2016

Patent Number: US Patent 20160149138A1

Flexible, printed electronics is a revolutionary new concept for fabricating optoelectronic devices using high-throughput, inexpensive solution processes (e.g., printing methodologies) on flexible plastic foils, which contrasts sharply with the highly specialized and expensive facilities and equipment required for silicon fabrication. By developing new electronic materials, these technologies can enable inexpensive, lightweight, flexible, optically transparent, and unbreakable components for a wide variety of applications such as displays, cell phones, medical diagnostics, RFID tags, and solar modules, which then can be integrated with textiles, printed batteries, solar cells, aircraft or satellite structures, and the like. The enabling material component of all these technologies (among other essential materials) is the semiconductor where charge transport, light absorption, and/or light generation occur. To broaden device functionalities and applications, two types of semiconductors are required: p-type (hole-transporting) and n-type (electron-transporting). The use and combination of these two types of semiconductors enable the fabrication of elementary electronic building blocks for driving displays, harvesting light, generating light, carrying out logic operations, and sensor functions. To enable high device efficiencies such as large charge carrier mobilities (μ) needed for transistor/circuit operations, or efficient exciton formation/splitting necessary for photonic devices, organic semiconductors should have an appropriate electronic structure to favor specific functions.

Software

χ-DB Database

J. De Pablo, I. Foster, D. Audus

Link: http://pppdb.uchicago.edu/

This digital handbook of properties contains 388 χ values for 120 polymers, 30 solvents. It includes 237 χ values for polymer blends of 63 unique polymers, which exceeds the 134 χ values for polymer blends of 41 unique polymers found in the Physical Properties of Polymers Handbook. The χ DB digital handbook also includes 84 newly published/measured χ values measured from 2010 to 2015 while the handbook was last published in 2007. Results of this work has been published in the Procedia Computer Science [25.3] and Journal for Chemical Education [25.4]

7.6 Publications and Presentations

7 Number of CHiMaD-supported publications in 2016 by Organic Bulk Heterojunction Polymer Solar Cells use-case group. Please see chapter 25 for details [25.17, 25.25, 25.32, 25.33, 25.34, 25.35, 25.36].

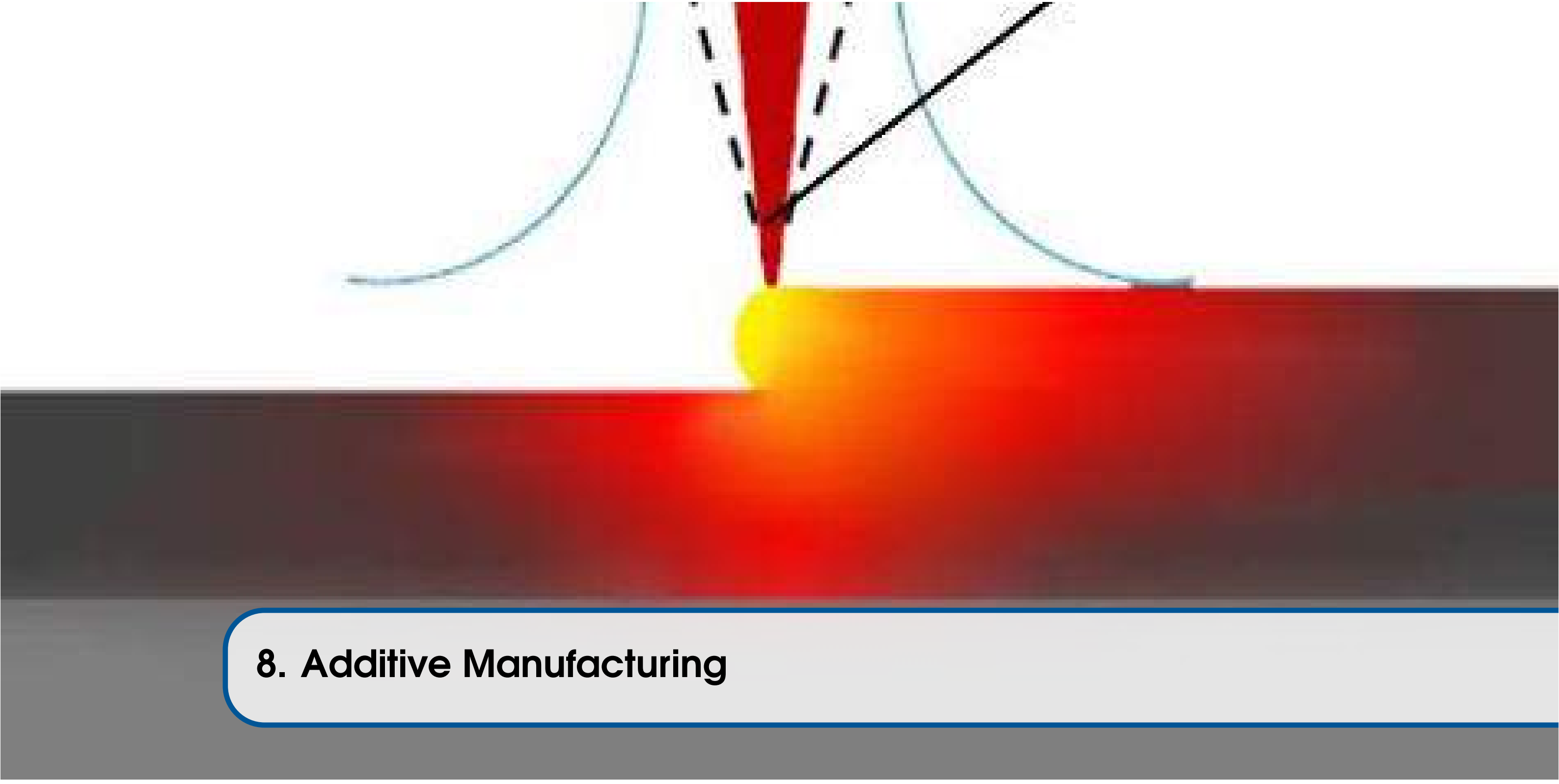
15 Number of presentations on CHiMaD supported research in 2016, please see section 24.11 for the complete list.

7.7 CHiMaD Team

Organic Bulk Heterojunction Polymer Solar Cells Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Luping Yu	Principal Investigator	UC/CHEM	
Juan de Pablo	Principal Investigator	UC/IME	
Guilia Galli	Principal Investigator	UC/IME	
Tobin Marks	Principal Investigator	NU/MSE	
Matthew Goldey	Postdoctoral Researcher	UC/IME	Electronic structure models of semiconducting small molecules and polymers for organic photovoltaics *(Galli)*
Ferdinand Melkonyan	Postdoctoral Researcher	NU/CHEM	Sulfonamide Organic Photovoltaic Building Blocks; Diacetylenes as Organic Photovoltaic Building Blocks *(Marks)*
Daniel Reid	Graduate Student	UC/IME	Simulation of OPV materials *(de Pablo)*
Alexander Schneider	Graduate Student	UC/CHEM	Organic bulk heterojunction polymer solar cells *(Yu)*
Qinghe Wu	Graduate Student	UC/CHEM	Electron Accceptors *(Yu)*

III

CHiMaD Seed Groups



8. Additive Manufacturing

Jian Cao (NU)

Lyle Levine (NIST), Li Ma (NIST), Carelyn Campbell (NIST), Mark Stoudt (NIST)

8.1 *Significance & Research*

Additive manufacturing breaks three fundamental manufacturing tradeoffs: capital versus scale, capital versus scope, and capital verses complexity. It also significantly reduces material waste by placing materials only where needed. Widespread acceptance of additive manufacturing will increase supply chain efficiency, reduce time to market, move from mass production to mass customization, and sustain the environment. This will spur a technology renaissance by bridging manufacturing of all scales with material design and will broaden participation by disseminating accessibility to cutting-edge manufacturing processes.

One area of interest for additive manufacturing via laser deposition is the repair of high cost cast iron components used in agricultural, automotive, and heavy equipment engines. The main difficulty in laser cladding on cast iron is the high level of cracking in the material because of its brittle nature. To reduce cracking, the temperature gradient formed during the laser deposition process should be kept as small as possible. Preheating reduces the thermal gradient which slows the cooling rate of the deposition and the region surrounding the deposition. Heating the entire workpiece in a furnace is most beneficial due to the uniform temperature distribution, but cannot be integrated into the laser deposition process without extreme modification to the laser deposition machine tool system or the addition of costly auxiliary equipment.

The implementation of heating and cooling rate control was investigated with the goal of enabling the multi-material repair of cast iron components via laser deposition. The primary goal of this work is to eliminate crack formation as a result of the thermal shock induced by the metal deposition process. For this purpose, an experimental investigation was conducted through the repair of a heavy duty diesel engine component. The feasibility of utilizing the laser to preheat the substrate and slow cooling after deposition was comprehensively investigated as a means of reducing cracking induced by thermal stresses.

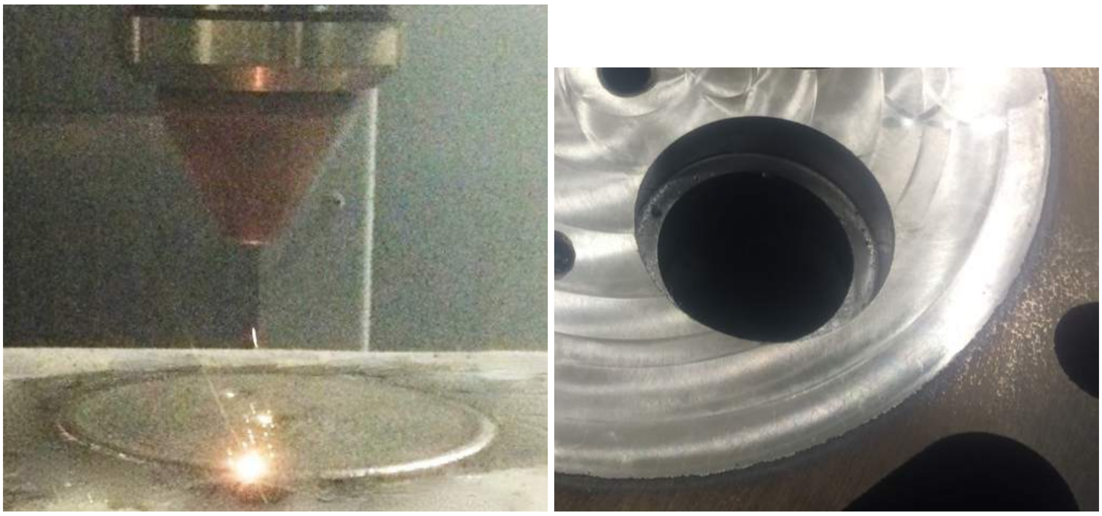


Figure 8.1: From Left to Right: (A) Laser deposition repair process (B) Completed Laser deposition repair

The volume to be repaired in the component was prepared by milling away the damaged area. The repair was then conducted by depositing nine successive layers of material into the machined pocket, as seen in Figure 8.1A. Stainless steel 316L was used as the deposited repair material. After deposition, the repaired surface was faced to be completely flat and true with the top surface of the component. In the uncontrolled trial, the laser deposition process was performed on a room temperature substrate without preheating or reheating. During subsequent trials, the processing area was preheated prior to deposition and the deposition was reheated to slow the cooling rate.

In the uncontrolled trial, the thermal shock induced by the repair caused the cast iron to crack at the perimeter of the heat affected zone around the entire circumference of the outside of the laser deposited repair area. The best preheating trial effectively reduced the maximum heating rate during the first deposition layer to 7.8 K/min and the average heating rate to 3.4 K/min, approximately halving the uncontrolled heating rate, and the application of the reheating cycles actively reduced the cooling rate from the uncontrolled rate of 6.7 K/min to 1.4 K/min. A comparison of the thermal history of the uncontrolled deposition versus the thermal history of the controlled deposition can be seen in Figure 8.2.

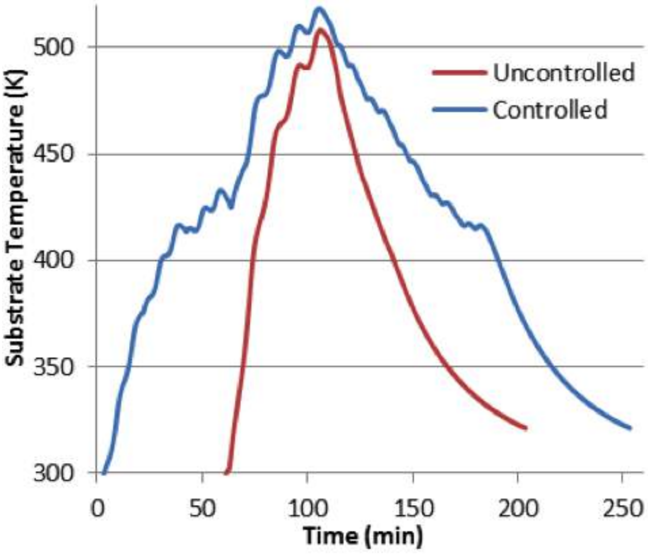


Figure 8.2: Uncontrolled and controlled process

This methodology successfully enabled a crack-free laser deposited repair of the cast iron diesel engine component, as seen in Figure 8.1B. All completed repairs were visually inspected for cracks under a microscope at 200x magnification. No cracks were observed on the repair that utilized the ideal set of preheating parameters and reheating parameters. Based on the absence of cracking, for this application, the repair was deemed a success. The successful repair of this component has demonstrated that preheating a reheating can be accomplished without extreme modification to the laser deposition system or the use of auxiliary equipment and that the deposition laser can be used to control temperature in laser deposition processes.

8.2 Collaborations

8.2.1 CHiMaD Collaborations

Additive Manufacturing of Co-Alloys

*Jian **Cao** (NU), Gregory **Olson** (NU), Wing-Kam **Liu** (NU)*

The graduate students from the three groups are working in collaboration on the topic of additive manufacturing.

8.2.2 NIST Collaborations

Additive Manufacturing

*Jian **Cao** (NU), Lyle **Levine** (NIST), Li **Ma** (NIST), Carelyn **Campbell** (NIST), Mark **Stoudt** (NIST)*

There is an active communication and exchange of research findings between these groups.

NIST Additive Manufacturing Workshop: Measurement Science for Directed Energy Deposition

*Jian **Cao** (NU), Lyle **Levine** (NIST), Li **Ma** (NIST), Carelyn **Campbell** (NIST), Mark **Stoudt** (NIST)*

This workshop was co-organized by the Additive Manufacturing use-case group and NIST colleagues at Northwestern University, Evanston, IL, USA on May 23-24, 2016.

8.2.3 External Collaborations

Collaboration with DMG-MORI USA

*Jian **Cao** (NU)*

An industrial collaboration on machine control has been established with *DMG-MORI, USA*, worth over \$1B.

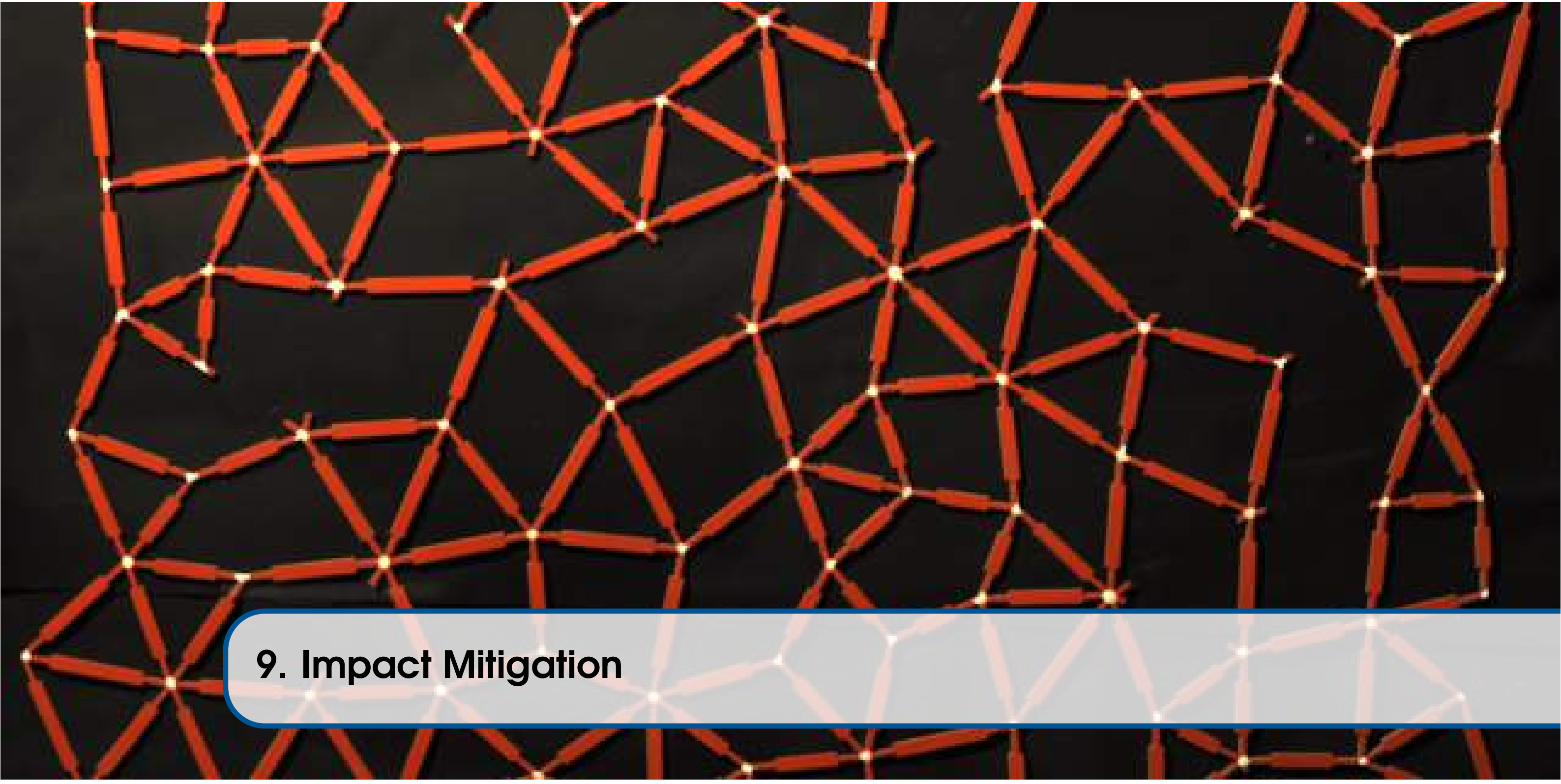
8.3 Publications and Presentations

2 Number of CHiMaD-supported publications in 2016 by Additive Manufacturing seed group. Please see chapter 25 for details. [25.21, 25.22]

2 Number of presentations on CHiMaD supported research in 2016, please see section 24.4 for the complete list.

8.4 CHiMaD Team

Additive Manufacturing Seed Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Jian Cao	Principal Investigator	NU/ME	
Jennifer Bennett	Graduate Student	NU/ME	Control of Additive Manufacturing *(Cao, Ehmann (NU))*



9. Impact Mitigation

Heinrich Jaeger (UC), Sidney Nagel (UC), Juan de Pablo (UC)

Aaron Forster (NIST), Chealsea Davis (NIST), Christopher Soles (NIST)

9.1 Significance & Research

The damaging effects of blunt impact on human physiology and health have been most notable in the manifestation of the high rates of chronic traumatic encephalopathy (CTE) in athletes, particularly football players. While this is the focus of current sports injury prevention, impacts to soft tissues are the basis for many chronic joint and musculoskeletal diseases. In team sports athletes rely on pads of geometrically structured, non-linear, time-dependent polymeric materials (e.g. elastomers, foams, thermoplastics, gas bladders, etc.), to absorb energy, limit momentum transfer, and reduce force at velocities that can exceed 45 m/s and energies up to 75 J. In many cases such materials are clearly inadequate, and there is a pressing need to reduce impact injuries to the head and body from a wide variety of threats in sporting, industrial, and military applications. Advances in protective materials have been incremental due to a lack of dynamic material property data and a lack of predictive models to spur innovation. The design goals of this Seed group are to develop innovative materials for impact mitigation that will be superior to those available today, and to do so by relying on predictive models coupled to high-precision experimentation in the context of both liquid and solid shock absorbing systems.

Design Principles for Novel Impact-Mitigating Materials

The **Jaeger** (UC), **Nagel** (UC) and **de Pablo** (UC) groups are developing the fundamental design principles for new materials that can effectively dissipate low-velocity impact, such as experienced during sport activities, where a major concern is that multiple impacts can lead to traumatic brain injury.

In collaboration with **de Pablo** (UC), **Jaeger** (UC) group is leading a systematic investigation of optimizing energy dissipation in dense suspensions; materials that can dynamically transform between solid- and liquid-like states and have highly effective energy absorption properties. This investigation couples detailed experiments with state-of-the-art simulations

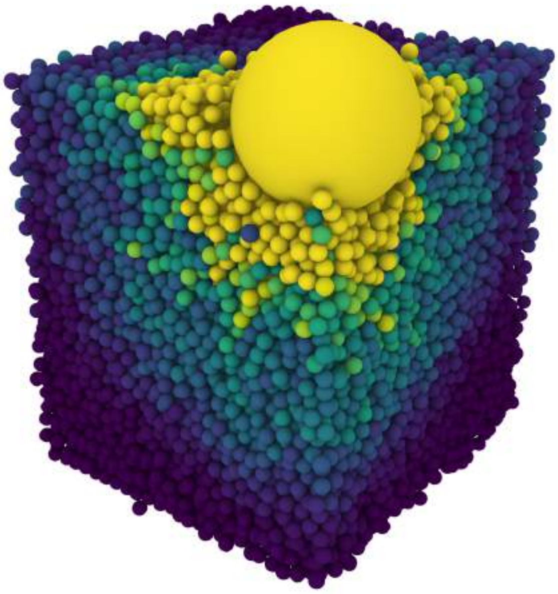


Figure 9.1: A snapshot from the new simulation code, showing a spherical impactor indenting a three-dimensional granular medium, with colors indicating the magnitude of the contact forces between neighboring particles (the image shows a corner cut through the 3d granular medium to better highlight the stress penetration, the simulated material extends beyond the corner; colors: yellow to blue = high to low contact force magnitudes)

to extract, for the first time, the materials parameters characterizing the stress-dependent particle-level interactions during impact.

In a second line of approach, the **Jaeger** (UC) group has initiated extensive simulations on dry granular materials with the goal of identifying the particle shapes and material architectures that are optimized for energy dissipation. This new simulation code, written and implemented in 2016, is based on Sandia Laboratory's LAMMPS platform for molecular dynamics simulations, see Figure 9.1. In 2017, this code will be combined with the evolutionary optimizer developed earlier by the **Jaeger** (UC) group.

Development of Innovative Materials Strategies

Recent advances in designing meta-materials have demonstrated that global mechanical properties of disordered spring networks can be tuned by selectively modifying only a small subset of bonds. Using a computationally-efficient approach, the**Nagel** (UC) group extended those results in order to tune more *general properties* of networks. This targeted behavior is reminiscent of the long-range coupled conformational changes that often occur during allostery in proteins.

With nearly complete success, the **Nagel** (UC) group is able to produce a strain between any pair of target nodes in a network in response to an applied source strain on any other pair of nodes by removing only 1% of the bonds. It is also possible to control multiple pairs of target nodes, each with a different individual response, from a single source, and to tune multiple independent source/target responses simultaneously into a network (Figure 9.2. Physical networks in macroscopic two- and three-dimensional systems that exhibit these responses have been fabricated. The simulations by the **Nagel** (UC) group

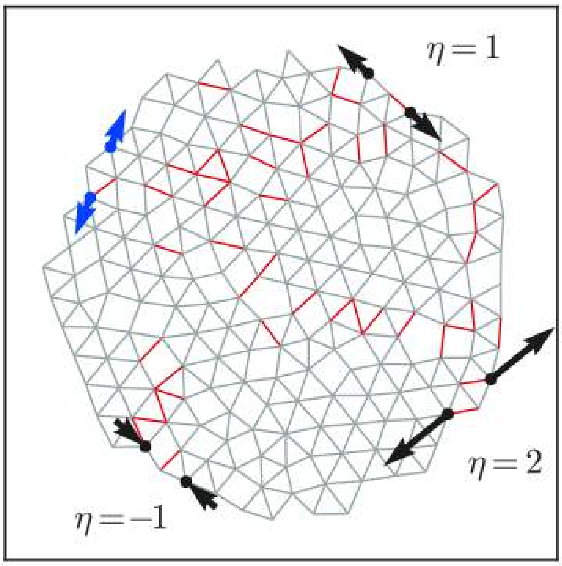


Figure 9.2: Network with 200 nodes and 502 bonds with an average coordination number of 5.0. The network was tuned to show responses at three target sites (shown by the black arrows) with responses of $\eta = 1, 2 and - 1$ where η is the ratio of the output to the input strain. All three targets are controlled by a single pair of source nodes shown by the blue arrows.

showed that the removal of a small number of bonds in a random elastic network can dramatically change its mechanical response. This theoretical approach precisely and efficiently controls the local strain at one point in such a network in response to a strain applied elsewhere in the system. The responses that were created are inspired by the long-range-correlated deformations that often characterize allostery in proteins. The ease with which these responses are created may give insight into *why* allostery is a common means for the regulation of activity in biological molecules.

Meta-materials consisting of networks attached by central-force springs can be created with specific designed properties. The**de Pablo** (UC) and **Nagel** (UC) groups are currently working towards generalizing this to situations where the interactions between nodes of the network include bond-bending forces. If successful, this would make the previously obtained results applicable to material networks consisting of mechanical struts between nodes. Such struts would necessarily have bond-bending forces at each node. The seed group aims to be able to create networks fabricated in two dimensions out of laser-cut sheets or in three dimensions using 3D printing which would exhibit the designed arbitrary properties

NIST-CHiMaD Impact Mitigating Materials for Body Protection Workshop

On August 8, 2016 CHIMaD and NIST hosted an Impact Mitigating Materials for Body Protection Workshop at the University of Chicago. This intimate workshop, 30 attendees, brought together leaders from academia and government in the areas of biomechanics, high-rate impact testing, and standard test methods for protective equipment. The workshop goals were to:

1. Identify current state-of-the-art in test-method development and injury thresholds
2. Identify methodologies to correlate material structure and dynamic properties to performance improvements from blunt impacts, ballistic, and blast protection
3. Identify ways Materials by Design concepts could accelerate innovation and reduce

injury rates

There were seven invited presentations in the morning broken into two sessions. The first session focused on the latest test methods for evaluating helmet performance in military and sports applications, with a presentation on innovative methods to structure materials to improve ballistic performance. The second session focused on the methodology used to understand an injury mechanism, experimentally recreate/validate the mechanism, and transition to a standard test method. The example injury was Commotio Cordis, a blunt impact to the heart that is rare in occurrence, but a high probability of fatality.

Overview of NIST and CHIMaD Perspectives on the Structure of a Materials-by-Design Approach to Address the Presented Challenges

Materials-by-Design approach is composed of novel dynamic-impact metrologies and novel, engineered energy-dissipation mechanisms for multi-material systems that are supported by new materials models. This perspective was a template for the afternoon group discussion topics:

- Injury Criterion and Ideal Material Response
  The biomechanics community has identified injury criterion for peak linear and rotational acceleration to reduce the risk of Traumatic Brain Injury (TBI). An ideal material should prevent head accelerations from reaching those limits in addition to meeting other design restrictions. Injury is subject to impact and biological conditions (age, neck strength, skull shape, etc.). Thus assessing protection requires balancing acceptable risk with the level of protection the material system can provide. The injury criterion for mild TBI is lower, but the injury criterion is not well defined and this is a challenge for developing protection systems.

- Measurement Strategies for Material Properties and System Performance
  The group identified better dynamic property measurements of materials as a need. There are several experimental dynamic metrologies (Kolsky, pendulum, drop tests, etc.) for materials and systems. These require trade-offs to optimize the test for the material or impact dynamics. Dynamic metrologies have unique challenges related to properties of soft, structured materials and a focused effort on soft material metrologies is required.

- Materials by Design
  This discussion identified a disconnect in the understanding of what materials work and why - specifically the influence of molecular architecture and interface behavior on dynamic response. Improvements in dynamic metrologies facilitate more accurate material models for elastic, nonlinear, time- and strain-sensitive material properties. Models of molecular and interface dissipation mechanisms will require new strategies to integrate them into the coarse finite element models used to simulate system and biological response to impacts. If done properly, material scientists and engineers can target the material architecture and structure to deliver a specific protection level.

9.2 Collaborations

9.2.1 CHiMaD Collaborations

Design of Novel Impact-Mitigating Materials

*Juan **de Pablo** (UC), Sidney **Nagel** (UC), Heinrich **Jaeger** (UC)*

The collaboration aims to develop design principles for new materials that can effectively dissipate low-velocity impact, such as experienced during sport activities, where a major concern is that multiple impacts can lead to traumatic brain injury.

9.2.2 NIST Collaborations

Development of Novel Metrologies

*Chelsea **Davis** (NIST), Aaron **Foster** (NIST), Juan **de Pablo** (UC), Sidney **Nagel** (UC), Heinrich **Jaeger** (UC)*

Complementing the NIST efforts lead by **Davis** (NIST) and **Foster** (NIST), the seed-group is developing metrologies for multiaxial dynamic loading coupled with distributed force measurement, and volumetric exterior strain measurements; the **Jaeger** group developed non-invasive, high-speed ultrasound imaging techniques to track the evolving, three-dimensional displacement field inside soft materials during impact.

NIST-CHiMaD Workshop on Impact Mitigating Materials for Body Protection

*Juan **de Pablo** (UC), Chelsea **Davis** (NIST), Aaron **Forster** (NIST), Sidney **Nagel** (UC), Heinrich **Jaeger** (UC)*

This one-day workshop brought together leading experts to discuss injury criteria and ideal material response characteristics with the aim to develop measurement strategies for desirable material properties and system performance in order to create novel impact mitigating materials by design. The workshop featured seven invited speakers from ARL, Virginia Tech, Johns Hopkins, UCLA, Carleton, Under Armour, and the Consumer Safety Commission as well as speakers from NIST and UC.

9.2.3 External Collaborations

Allosteric Response in Networks

*Sidney **Nagel** (UC), Andrea Liu (University of Pennsylvania)*

This collaboration focuses on developing efficient algorithms to design allosteric response into networks that have been created from jammed packings. The results of this collaboration has been published in PNAS [25.28].

9.3 Publications and Presentations

4 Number of CHiMaD-supported publications in 2016 by Impact Mitigation seed group. Please see chapter 25 for details. [25.18, 25.19, 25.20, 25.28]

7 Number of presentations by Impact Mitigation seed group in 2016, please see section 24.8 for the complete list.

9.4 CHiMaD Team

Impact Mitigation Seed Group Researchers			
Name	**Position**	**Affiliation**	**Project** (PI)
Juan de Pablo Sidney Nagel Heinrich Jaeger	Principal Investigator Principal Investigator Principal Investigator	UC/IME UC/PHY UC/PHY	
Nidhi Pashine	Graduate Student	UC/PHY	Designing allostery-inspired response in mechanical networks *(Nagel)*
Daniel Reed	Graduate Student	UC/IME	Designing user-specified mechanical responses in network based materials *(de Pablo)*

IV

CHiMaD Tools & Facilities

MATERIALS
DATA
FACILITY

10. Materials Data Facility

Ian Foster (UC/ANL), Steven Tuecke (UC/ANL), Benjamin Blaiszik (UC/ANL)

Chandler Becker (NIST), Sherif Youssef (NIST), Alden Dima (NIST), Robert Hanisch (NIST), Mary Brady (NIST), Raymond Plante (NIST), Zachary Trautt (NIST), Kimberly Tryka (NIST), James Warren (NIST), Carelyn Campbell (NIST), Martin Green (NIST), Aaron Kusne (NIST), Nhan Nguyen (NIST)

Significance

In 2016, the Materials Data Facility (MDF) deployed into production and operated a data publication service that allows researchers to self-publish datasets ranging in size from the very small, to very large (i.e., many-TB or millions of files) in size, while also exposing flexible data sharing and search capabilities for these published datasets. Work also began on development of a search index to promote discovery of materials science data that may be stored in diverse locations, comprised of diverse dataset collections, or encoded in heterogeneous data formats. As these services continue to advance, these capabilities will allow CHiMaD researchers to automate sharing of results internally and then broadly share published results with the public and other researchers in the community. These capabilities will also help NIST MGI goals by making datasets generated via CHiMaD, select NIST resources, and other community datasets more discoverable, more simple to share, and more accessible via standard web protocols.

10.1 Design Goals

The high-level goal of the Materials Data Facility project is to build a suite of data services and tools to make materials data more easily publishable and discoverable, and to decrease the barriers inherent to sharing and describing complex and often large materials science datasets. These services will be operated in the cloud to allow researchers to access the advanced capabilities without the burden of installing and maintain complicated software packages.

The goals of the MDF project include delivering data publication and data discovery capabilities to researchers while managing these capabilities as scalable production services for the materials community. More specifically, MDF aims to:

- Deliver publication capabilities to initial materials communities with a special focus on allowing publication, sharing, and description of datasets with metadata for both large (i.e., large by number, diversity, or size) and small datasets

- Build a search index to expand and augment current capabilities to allow researchers to discover and access datasets (and results within datasets) with limited information via free text search, fuzzy matching, range queries, browsing, and faceting of results.

10.2 Accomplishments in Research and Features

10.2.1 Data Publication

The MDF Data Publication Service (MDF-DPS) opened to limited release in January 2016, and to CHiMaD researchers and the general materials community in late February of 2016. MDF-DPS has been integrated with the core *Globus* services of authentication, user groups, sharing, and transfer. These integrations allow the MDF-DPS web user interface (UI) and API access to: advanced file sharing capabilities for reliable, secure, verified, and highly-optimized movement of data with sizes ranging from kB to PB; authentication tools to allow MDF users to authenticate with existing institutional credentials (e.g., user@northwestern.edu); user group tools that allow for dynamically limiting dataset access to a set of defined users; and sharing tools that allow data sharing and publication directly from campus servers, laptops, or national compute resources.

REST API and Python Client Support

API support, expanded from MDF's web-based user interface, will allow researchers to automate data publication, bulk deposit datasets, and will allow MDF to more easily interface with a variety of external services. To support automated publication of datasets integrated with current workflows, we have created REST-based APIs for creating and inspecting MDF datasets as well as tools for using the API from a command line interface or in custom scripts.

The REST API uses the Globus Authentication service to identify all users making API calls, just as with MDF web interface. This results in dataset and collection visibility being consistent between access modes (web UI, API), and also creates properly attributed datasets when they are submitted using the API. The API itself allows listing of all schemas, collections, and communities within the MDF with input and output data represented in the JSON format. This allows programmatic browsing of the contents of the MDF. Further, descriptive metadata (including Globus links to the underlying files) for individual datasets may also be retrieved using the API.

The REST API also allows for creation of new datasets. Creation occurs in a two-phase manner. In the first phase, the user provides the descriptive metadata, and the dataset entry is made in the MDF. During this first phase, MDF allocates a storage location for the dataset and returns this location to the user. The user is free to take as long as necessary (i.e., asynchronously assemble the dataset) to populate the storage location with their dataset contents using Globus Transfer. When the data transfers are complete, the user executes the second phase, indicating that the dataset is ready for final publication. Should the user prefer, they may switch to the web interface between phases one and two to view their in-progress dataset and interact with, inspect and edit details, and ultimately submit the dataset via the web UI.

Command Line Access

The REST interface has been wrapped with a command line utility for executing many of the functions of the REST API. This includes basic queries to introspect and browse the state of the MDF data publication service, as well as single command functions that perform the entire workflow to create a new dataset, including the required transfer operations. This utility not only simplifies access to the interface, but it also allows easy integration with other scripting use cases.

Results

To bootstrap usage of the MDF-DPS, we have allocated 100 TB of staff-managed, reliable storage resources to support early adopters in the CHiMaD project and open data sharing of materials science datasets of broader interest to the community.

During our first 12 months of operation, a variety of high value datasets to the community were published representing 24 individual datasets from researchers associated with 9 academic institutions and national laboratories with data volume comprising *6.7 TB of raw data*. Datasets published by MDF have been accessed over *1000 times* by users in the last 6 months.

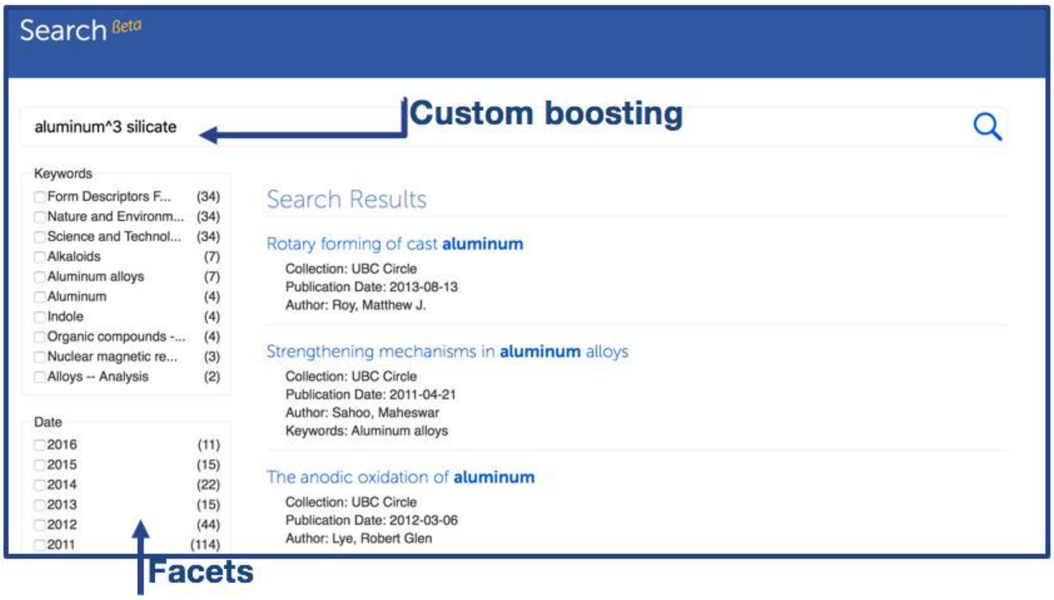
10.2.2 Data Discovery

As more materials data is published with the Materials Data Facility and other distributed services, discovery of datasets, subsets of datasets, or results from datasets becomes a more challenging problem. These problems become even more challenging as dataset diversity increases since researchers may want to filter and facet based on queries that are scientifically relevant to their specific field. To this end, we are addressing this problem by building a dedicated, highly-scalable, flexible, domain-agnostic index of research data. Key characteristics of this index are:

- **Domain agnostic:** The index will allow datasets to be described using terminology that is most appropriate to the domain or scientific practice of its publisher and users. This is in contrast to many indexes that are purpose built for a particular community or scientific vocabulary. While extensible in this way, the index will also support and steer users to common schemas (such as basic Dublin Core and especially NIST derived materials schemas) where appropriate and available.

- **Powerful search capabilities:** The search interface supports powerful query syntax. While basic free text based searching is possible, it is also possible to search by property values, ranges of values (for both numeric and date values), or perform fuzzy and wildcard matching, see Figure 10.1.

- **Faceted overlays:** As the volume of searchable data increases, filtering and browsing becomes a more valuable means of discovering relevant results. Our search index supports faceting: tabulation of counts on the number of documents matches for certain search terms. However, unlike many other indices, the set of facets is dynamic and may be specified on a per-query basis. This allows the facets to overlay the basic



aluminum^3 silicate

Keywords	
☐ Form Descriptors F...	(34)
☐ Nature and Environm...	(34)
☐ Science and Technol...	(34)
☐ Alkaloids	(7)
☐ Aluminum alloys	(7)
☐ Aluminum	(4)
☐ Indole	(4)
☐ Organic compounds -...	(4)
☐ Nuclear magnetic re...	(3)
☐ Alloys -- Analysis	(2)

Date	
☐ 2016	(11)
☐ 2015	(15)
☐ 2014	(22)
☐ 2013	(15)
☐ 2012	(44)
☐ 2011	(114)

Search Results

Rotary forming of cast **aluminum**
Collection: UBC Circle
Publication Date: 2013-08-13
Author: Roy, Matthew J.

Strengthening mechanisms in **aluminum** alloys
Collection: UBC Circle
Publication Date: 2011-04-21
Author: Sahoo, Maheswar
Keywords: Aluminum alloys

The anodic oxidation of **aluminum**
Collection: UBC Circle
Publication Date: 2012-03-06
Author: Lye, Robert Glen

Figure 10.1: Screenshot from our internal beta search index (test data indexed). The search capabilities support fuzzy match, partial match, custom boosting, custom faceting of results, and per-indexed-item access control lists.

search and help the user narrow results to values that are particularly prominent or significant.

- **Access controlled:** Each indexed entry may contain information specifying individual or groups of users that are permitted to view the information. Multiple sets of metadata may be applied to a single dataset with different permissions allowing for different users to see different views on a single dataset depending upon those permissions. This promotes an open, participatory environment where various users can contribute to the description of a dataset with assurance that only other desired users can see that description. This is particularly useful in, for example, embargo scenarios.

An important goal of this new search index service is to integrate and expose existing feeds and diverse streams of data as readily as possible while respecting access control permissions. Our approach to this is three-fold: first, as stated previously, we do not specify or require any specific schema for the metadata, though we encourage use of relevant standards where applicable. Second, we use a small, flexible wrapper format to define the target, syntax, and visibility of metadata while retaining the bulk of the metadata in its native format. Third, since the metadata is specified in a file to be indexed, a physical copy of the metadata is maintained in proximity to the data it describes and in the cloud index.

We expect to interface with a broad set of CHiMaD-affiliated research groups and use cases as well as national materials science efforts in the coming six months to further populate and test our search index capabilities.

10.3 Access Information and Status

Data publication services are now available to CHiMaD researchers and researchers in the broader materials community. Researchers interested in using MDF services within their personal research, research group, or larger collaborations can visit *www.materialsdatafacility.org* for more information or contact the MDF project PIs. A "Quick Start" documentation is available at *https://github.com/globus/mdf*.

10.4 GlobusWorld Tour

During 2016, the MDF team has also kicked off the *GlobusWorld Tour* series (with accompanying webinars) that focused primarily on helping developers and researchers understand and leverage the core *Globus* services, but also covered aspects of data publication, data discovery, and highlighted MDF as a specific use case. Four presentations were given to date, please refer to Section 24.7 for details.
Globus 101 Webinar: *https://www.youtube.com/watch?v=K17ZZEIvWhg*

10.5 Collaborations

10.6 NIST Collaborations

High-throughput Experimental Materials Science Virtual Laboratory
Ian ***Foster*** *(UC/ANL), Benjamin Blaiszik (UC), Zachary* ***Trautt*** *(NIST), Martin* ***Green*** *(NIST), Aaron* ***Kusne*** *(NIST), Nhan* ***Nguyen*** *(NIST)*
MDF will take part as a node in the Materials Science Virtual Laboratory (MSVL) that is led by NIST. The MSVL will leverage MDF and other *Globus* services to provide key aspects of the data infrastructure for the evolving project.

Ingest of Materialsdata.nist.gov Data into MDF Data Publication and Discovery Services
Ian ***Foster*** *(UC/ANL), Benjamin Blaiszik (UC), Carelyn* ***Campbell*** *(NIST)*
Collaborating with **Campbell** (NIST), MDF is investigating cross-hosting and/or indexing of datasets available currently on *materailsdata.nist.gov* to improve access and discoverability. We are also investigating the advantages deeply indexing dataset contents into our search index to provide a search interface to results from a portion of the datasets.

Cloud Deployment of a MDF Materials Resource Registry (MRR)
Ian ***Foster*** *(UC/ANL), Benjamin Blaiszik (UC), Laura Bartolo (NU), Chandler* ***Becker*** *(NIST), Sherif* ***Youssef*** *(NIST), Alden* ***Dima*** *(NIST), Robert* ***Hanisch*** *(NIST), Mary* ***Brady*** *(NIST), Ray* ***Plante*** *(NIST), Zachary* ***Trautt*** *(NIST), Kimberly* ***Tryka*** *(NIST), James* ***Warren*** *(NIST)*
Working with researchers at NIST, MDF has deployed an instance of the MRR software on Amazon Web Services. We are working to populate this instance with resources that may be especially important to researchers within CHiMaD and will allow cross-harvesting of our records with NIST in the coming 6 months.The MRR instance launched on MDF as part of CHiMaD efforts will be part an international Materials Data Federation.

10.7 External Collaborations

Integrative Materials Design: Midwest Big Data Spoke Joint Proposal
Ian ***Foster*** *(UC/ANL), Benjamin Blaiszik (UC), Laura Bartolo (NU), Peter* ***Voorhees*** *(NU),*

Dane Morgan (UW-Madison), John Allison (UM-Ann Harbor), Dallas Trinkle (UIUC)
This recently awarded collaborative proposal by materials researchers at UC, NU, Argonne, UIUC, UW-Madison, UM-Ann Arbor aims to connect various efforts across the Midwest, including industrial, to build a variety of partnerships and leverage shared data services and capabilities in their materials design and research efforts as part of the national Big Data program. In support of these efforts, the NSF created the IMAD (Integrative Materials Design) data respository. IMAD is the materials-focused Spoke on the Midwestern Big Data Hub that employs the MDF infrastructure.

10.8 Future Outlook

In 2017, we will greatly expand our efforts to index and publish datasets that are critical to the success of CHiMaD. We will build a variety of new functionality to support more complex MDF data publication and synthesis use cases (e.g., pipelines that combine theory and experimental data, more flexible metadata model for dataset description, and potentially data versioning) that have been uncovered during our initial interactions with CHiMaD researchers. We also expect to make available our data discovery service, populated with datasets from CHiMaD, results from broad spectrum of national materials-related efforts, as well as open data sources, to the community in 2017.

10.9 Technology Transfer

Data Services
Materials Data Facility
I. Foster, S. Tuecke, B. Blaiszik, K. Chard, J. Pruyne, M. Ondrajcek
Access Link: https://materialsdatafacility.org

Data
Datasets Uploaded to MDF by CHiMaD Principal Investigators in 2016
∗ denotes group permission is required to access the data

Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material $(PbSe)_5(Bi_2Se_3)_3$ [DOI: 10.18126/M2MS3W]
Data from CHiMaD Publication 25.12
X. Ren, A. K. ***Singh*** *(NIST), L. Fang, M. G. Kanatzidis, F.* ***Tavazza*** *(NIST), A. V.* ***Davydov*** *(NIST), L. J.* ***Lauhon*** *(NU)*

Rotationally Commensurate Growth of MoS_2 on Epitaxial Graphene* [DOI: 10.18126/M2G59Q]
Data from CHiMaD Publication 25.43
X Liu, H. Bergeron, M. ***Bedzyk*** *(NU), M.* ***Hersam*** *(NU) et al.*

Point Defects and Grain Boundaries in Rotationally Commensurate MoS_2 on Epitaxial Graphene* [DOI: 10.18126/M29G64]
Data from CHiMaD Publication 25.11
X. Liu, H. Bergeron, M. ***Hersam*** *(NU) et al.*

Anisotropic Thermal Conductivity of Exfoliated Black Phosphorus [DOI: 10.18126/M23W2W]
H. Jang, M. ***Hersam*** *(NU), D. Cahill et al.*

Liquid-solid Metallic Mixture Coarsening Data - 28% solid [DOI: 10.18126/M27P4T]
J. Gibbs, J. Fife, P. ***Voorhees*** *(NU)*

Liquid-solid Metallic Mixture Coarsening Data - 35% solid [DOI: 10.18126/M2059C]
J. Gibbs, J. Fife, P. ***Voorhees*** *(NU)*

Liquid-solid Metallic Mixture Coarsening Data - 55% solid [DOI: 10.18126/M2VC7F]
J. Gibbs, J. Fife, P. ***Voorhees*** *(NU)*

Liquid-solid Metallic Mixture Coarsening Data - 80% solid [DOI: 10.18126/M23W2W]
J. Gibbs, J. Fife, P. ***Voorhees*** *(NU)*

Ostwald Ripening of Faceted Si Particles in an Al-Si-Cu Melt [DOI: 10.18126/M2Z592]
A. Shahani, P. ***Voorhees*** *(NU) et al.*

Twin-mediated Crystal Growth: an Enigma Resolved [DOI: 10.18126/M2301J]
A. Shahani, E. B. Gulsoy, P. ***Voorhees*** *(NU) et al.*

The Mechanism of Eutectic Growth in Highly Anisotropic Materials [DOI: 10.18126/M26P4H]
A. Shahani, P. ***Voorhees*** *(NU) et al.*

Gravure Printing of Graphene for Large-Area Flexible Electronics* [DOI: 10.18126/M2F59D]
E. Secor, S. Lim, M. ***Hersam*** *(NU) et al.*

Inkjet Printing of High Conductivity, Flexible Graphene Patterns* [DOI: 10.18126/M2K01W]
E. Secor, B. Ethan, P. Prabhumirashi, M. ***Hersam*** *(NU) et al.*

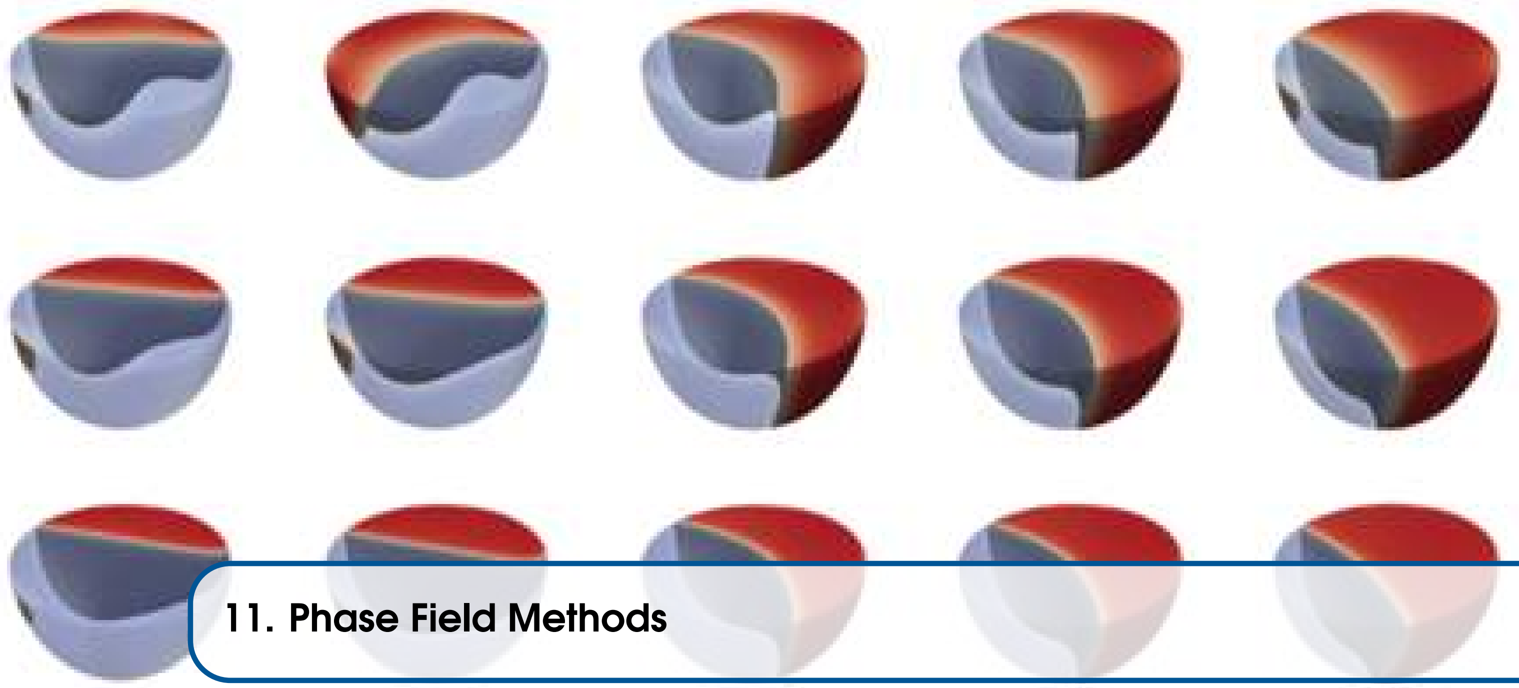
10.10 Publications and Presentations

1 Number of CHiMaD-supported publications in 2016 by Materials Data Facility Developers. Please see chapter 25 for details. [25.27]

14 Number of presentations on CHiMaD supported research in 2016, please see section 24.7 for the complete list.

10.11 CHiMaD Team

Materials Data Facility Developers		
Name	**Position**	**Affiliation**
Ian Foster	Principal Investigator	UC/CI
Steven Tuecke	Deputy Director	UC/CI - ANL/MCS
Benjamin Blaiszik	Software Developer	UC/CI - ANL/MCS
Kyle Chard	Senior Researcher/Fellow	UC/CI - ANL/MCS
Jim Pruyne	Senior Software Developer	UC/CI
Michal Ondrejcek	Research Programmer	UIUC/NCSA



11. Phase Field Methods

Olle Heinonen (NU), Peter Voorhees (NU), David Chopp (NU), Barry Smith (ANL)

James Warren (NIST), Jonathan Guyer (NIST)

Significance

Mesoscale materials modeling, that spans length and time scales larger than atomic but smaller than macroscopic, is central to modeling materials structural evolution. This is particularly the case for systems in which several degrees of freedom, such as elastic strain and diffusion, are coupled in inhomogeneous materials structures. Phase field methods are one set of mesoscale approaches to deal with such systems. CHiMaD is advancing phase fields methods with a goal of having quantitatively predictive modeling capabilities for structural evolution of three-dimensional systems. The efforts span both development of computational methods, algorithms, and models, as well as developing community standard problems for benchmarking, verification, and validation of phase field codes.

11.1 Research

11.1.1 Community Standard Phase Field Codes

Heinonen (ANL), **Voorhees** (NU), **Warren** (NIST) and **Guyer** (NIST), along with postdoctoral researchers Jokisaari (NU-ANL) and Keller (NIST), have brought together an elite team of Phase Field experts and framework developers during CHiMaD Phase Field Methods Workshops I-III. The goal of these workshops was to develop the first-set of benchmark problems for the global phase field community and to engage this elite team of invited experts for in providing input during this development. On that end, Hack-a-thons have been organized in Workshops II-IV where students, postdoctoral researchers and experts have gotten a chance to tackle the drafted benchmark problems. The first set of benchmark problems for the Phase Field community has been published in *Computational Materials Science* [25.30], and has been selected as the Editor's Choice (Figure 11.1). The published benchmark problems have been constructed based on the discussion and feedback during the CHiMaD Phase Field Workshops. The benchmark problems,

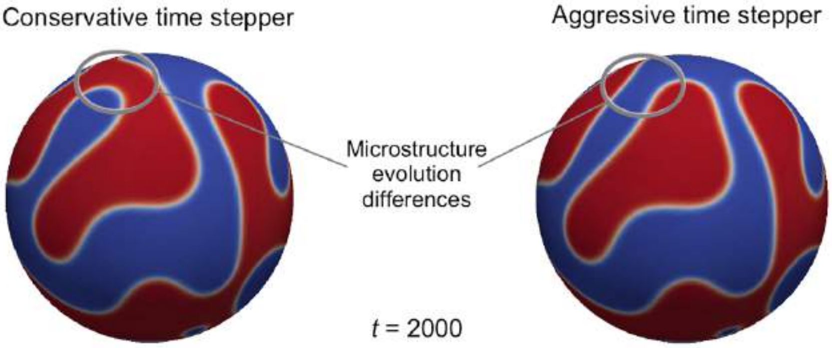


Figure 11.1: Snapshot of the microstructure evolution for spinodal decomposition on the surface of a sphere. The figure illustrates differences obtained with different time steppers at a snapshot in time: the left figure is generated using a conservative time stepper, and the right figure an aggressive time stepper.

together with one set of solutions, have been made available online for the community at the CHiMaD Phase Field Website developed by Wheeler (NIST) and can be accessed at *(https://pages.nist.gov/chimad-phase-field/#benchmarks)*. It is expected that these benchmark problems will be a significant resource for developers of phase field codes - the problems are already being used in college courses taught by CHiMaD Phase Field Methods workshop contributors such as by Michael Tonks (Penn State). A second set of benchmark problems are in preparation and will be tested in 2017 during CHiMaD Phase Field Methods workshops IV-V.

11.1.2 Investigation of Phase separation in an AlCrNi Alloy

Phase separation in an AlCrNi alloy was investigated with a phase-field model by **Voorhees** and Poulsen (NU). Growth and subsequent coarsening was simulated for an initial set of 510 γ' precipitates, see Figure 11.2. Initial precipitate size corresponded to the critical particle size, and simulation proceeded until the mean particle size had increased by a factor of 2. All thermodynamic and kinetic parameters were adapted from CALPHAD assessments with full compositional dependence, and integrated into the simulation without introducing additional approximations. The results were compared to experimental data, and provided evidence for precipitate coalescence as an important mechanism for early stage microstructural evolution. Phase-field models are increasingly applied to problems in materials science without consideration of the inherent assumptions. Current work probes the ubiquitous assumption of permanent equilibrium of the vacancy distribution, and attributes a significant discrepancy between the experimental and simulated rate of microstructural evolution to the violation of this assumption at the small length scales examined. Additionally, only few other examples of direct incorporation of CALPHAD databases into phase-field models of non-binary alloys are found in the literature. This must be considered a necessity for application of the phase-field method to commercially relevant alloys.

11.1.3 Application of Phase Field Methods to Complex Geometries

Two schemes for incorporating Dirichlet boundary conditions into diffusion-like partial differential equations in domains of complex geometries without introduction of non-

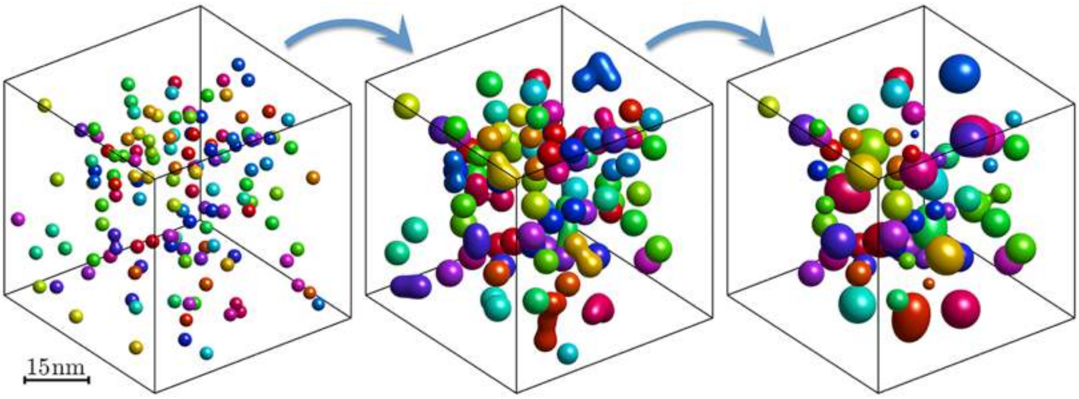


Figure 11.2: Growth of γ' precipitates in a γ matrix at times 1h10min (left), 3h32min (middle), and 19h00min (right) of aging time

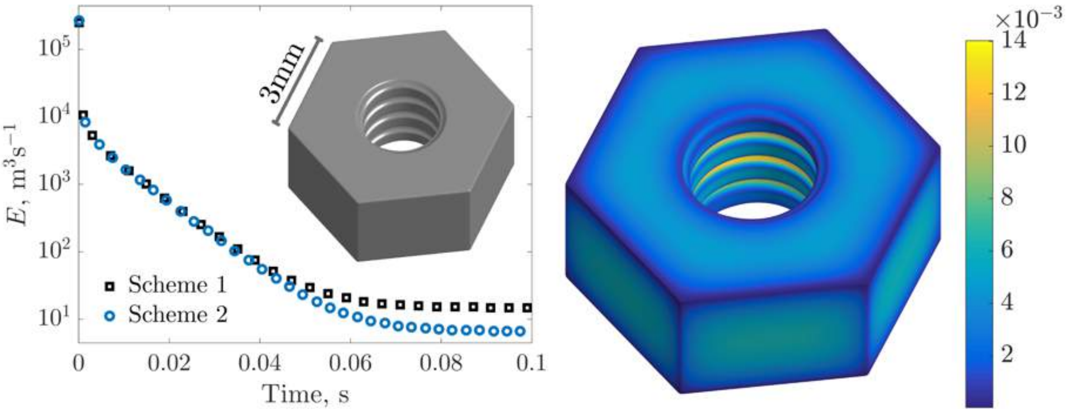


Figure 11.3: Energy functional of the two schemes during simulated heat transfer in an industrial component (left), relative deviation of the determined solution and the exact boundary condition at the component interface at t=15ms

Cartesian meshes were presented, see Figure 11.3, by **Voorhees**. These schemes were shown to correspond to energy penalty methods, and were guaranteed to converge to the exact solution in the limit where a model length scale is chosen sufficiently short relative to the feature size of the domain. It was shown that both schemes admit an additional model parameter which guarantees that deviations from the exact solution is confined to a small region near the boundary when chosen correctly. Since the presented methods are energy penalty methods, they may be straightforwardly incorporated into variational phase-field methods while ensuring that the energy (or entropy) functional will evolve monotonically (i.e. gradient stable), which is often the only available means to examine if a model and numerical solver is functioning as desired. The smoothed boundary method may be applied to a wide range of model types and numerical solution schemes, and is easily implemented computationally.

11.1.4 Investigation of Anisotropic Solid-Liquid Interfaces using Phase-Field Crystal Methodology

A continuum atomistic modeling formalism, the phase-field crystal methodology (PFC), has been employed to understand the properties of anisotropic solid-liquid interfaces. The method is capable of resolving atomistic length scales evolving over diffusive time scales. Thus far, for single component systems, Ofori-Opoku (NIST-NU), in collaboration with **Voorhees** (NU) and **Warren** (NIST) has investigated the capability and applicability of the model to solidification microstructures. It was found that the method is well suited for describing the surface energetics, modes of growth and kinetics of interfaces in the limit of vanishing interfacial width, as well as vanishing and negative interfacial stiffness. However, the method is limited to describing microstructures on atomistic length scales. To circumvent the atomistic length scale restriction in order to examine microstructural features at the mesoscale, coarse-graining procedures are being applied to the PFC model in attempts to generate diffusional models that operate on large length scales.

Through coarse-graining methods, PFC functionals can be smoothed to give models that operate on the mesoscopic length scales. The models resemble those models of conventional phase-field (PF) models, however now informed from and retaining atomistic scale features that allow for the self-consistent description of highly anisotropic surfaces. Using a particular form of coarse-graining, we have generated two variant archetypes of PF models. One, which resembles the multi-order parameter PF methods, and another which while allowing for multiple order parameters, also allows for the self-consistent description of topological defects, such as dislocations, and elasto-plastic effects. Using the former of these models, Ofori-Opoku (NIST-NU), **Voorhees** (NU) and **Warren** (NIST) have validated, through calculations of interfacial energetics, equilibrium shape via Wulff construction, and growth, that this higher length scale formalism indeed is capable of describing faceted surfaces without the need for additional ad hoc descriptions or additions of the form of the surface stiffness as is usually required in conventional PF models. In Figure 11.4, top row shows the surface energy (in polar form) as the system approaches the faceting transition with decreasing temperature from left to right. Also depicted in Figure 11.4, the bottom row is the corresponding equilibrium crystal shape, from a Wulff construction, clearly showing the emerging faceted shape. Evident in the latter temperature image is the emergence of rounded cusps in the surface energy plot and so-called ears in the Wulff construction, a hallmark of the appearance of corners on the Wulff shape. Being a coarse-grained model, note that the corners are rounded, in a manner consistent with the derived model, which generated a self-consistent regularization contribution to the free energy functional. The results obtained thus far are being prepared in the form of two separate manuscripts for publication. The researchers are now in the process of transferring this knowledge to

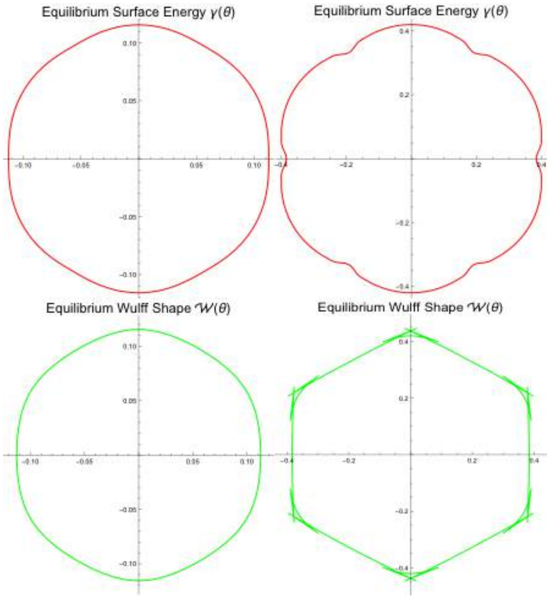


Figure 11.4: Equilibrium surface energy and Wulff Shape in polar coordinates. System temperature decreases from left to right, with the top row showing the surface energy while the bottom row shows the Wulff shape construction. Note the emerging cusps (rounded) in the surface energy and the accompanying emergence of ears in the Wulff construction.

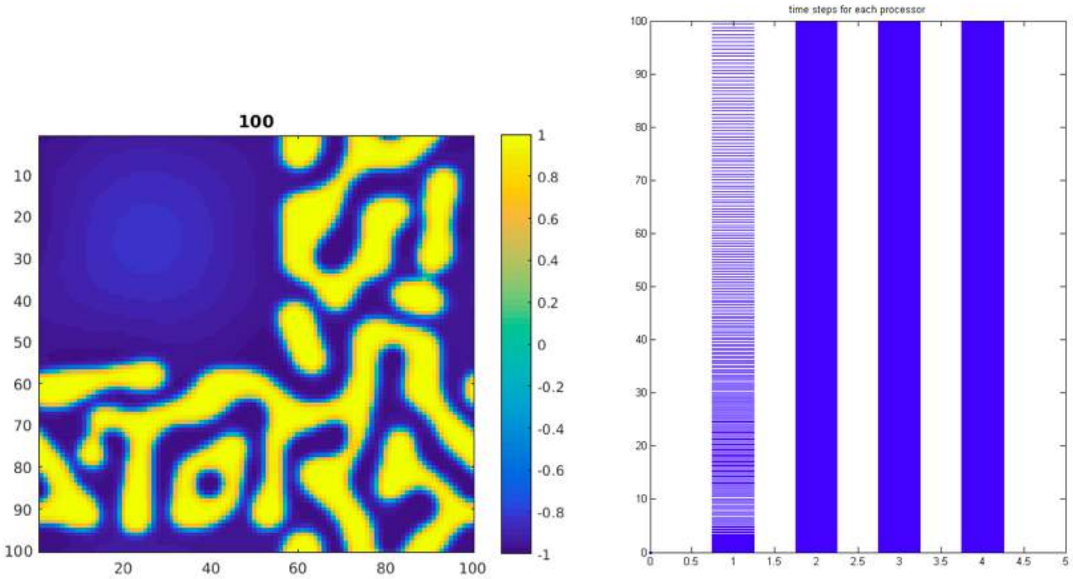


Figure 11.5: Left to right: (A) A single-phase test subdomain is shown while the other subdomains are initiated with random values.(B) Locations of time steps

the case of alloys with the aim of eventually investigating faceted structures in eutectics. Simultaneously, the behavior of the second of the variants of coarse-grained models derived from the PFC is also being examined.

11.1.5 Parallel Locally Adaptive Time Stepping (PLATS) Method

Chopp group has successfully developed a parallel locally adaptive time stepping (PLATS) method for the Cahn-Hilliard equation using a first order time-stepping algorithm. The PLATS method allows the domain to be subdivided into many subdomains, where each subdomain maintains its own time-step size, and neighboring subdomains are not required to synchronize temporally. **Chopp** group has shown that the same results are achieved using the PLATS method as the standard serial method. To illustrate the utility of this method, a single-phase test subdomain is shown in Figure 11.5A, while the other subdomains are initiated with random values. The upper left one-phase region is able to use a significantly larger time step compared with the other regions as illustrated by the locations of time steps marked in Figure 11.5B. The goal of developing the PLATS method is to have the ability to solve the Cahn-Hilliard equation for longer time intervals than existing methods. In 2017, a second order in time version of the PLATS algortihm is planned along with more realistic tests to demonstrate the effectiveness of the method. This is expected to complete the doctoral thesis work of Sereewattanawoot (NU) in **Chopp** (NU) group and be published.

11.2 Collaborations

11.2.1 Internal Collaborations

Modeling of Microstructural Evolution of Co-based Super Alloys

*Peter **Voorhees** (NU), David **Dunand** (NU), David **Seidman** (NU), Olle **Heinonen** (ANL), Christopher **Wolverton** (NU), Barry **Smith** (ANL)*

This collaboration focuses on complementing the efforts of the Precipitation Strengthened Alloys use-case group and utilizes phase field methods to determine the morphology of precipitates in Co alloys; a computational model for the equilibrium shape of γ' inclusions in a γ-phase matrix of Co-W-Al alloys. **Dunand** (NU), **Seidman** (NU), **Wolverton** (NU) groups provided the inputs such as interface structure, compositions, interfacial energies for the modeling lead by **Voorhees** (NU) and **Heinonen** (ANL) groups while **Smith** (ANL) was consulted for numerical and applied math issues that arose during the modeling.

Precipitation Strengthened Alloys

*Peter **Voorhees** (NU), Stephen **Davis** (NU)*

This collaboration focuses on developing models of rapid solidification of multicomponent alloys for use in additive manufacturing applications.

PLATS method for Cahn-Hilliard equation

*Peter **Voorhees** (NU), David **Chopp** (NU)*

Voorhees (NU) group will provide the **Chopp** (NU) group problems for validating their completed PLATS algorithm.

Modeling Precipitate Growth in Multicomponent Alloys

*Peter **Voorhees** (NU), David **Chopp** (NU)*

This collaboration focuses on developing models of precipitate growth in multicomponent alloys using the level set methodology. A code for Ostwald ripening for multi-component systems that uses fully resolved time for the diffusion rather than the standard quasi-steady state approach is being developed. Level set method will be used to track the solid domain boundaries, and a parallelized heat equation solver for the temporal diffusion.

Advanced Phase Field Methods

*Marius **Stan** (ANL), Olle **Heinonen** (ANL)*

This collaboration focuses on improving phase field models for predicting ionic transport in materials for energy storage applications (battery electrodes).

11.2.2 NIST Collaborations

Phase Field Benchmark Problems

*Olle **Heinonen** (ANL), Peter **Voorhees** (NU), James **Warren** (NIST), Jonathan **Guyer** (NIST)*

This collaboration, along with postdoctoral researchers Jokisaari (ANL) and Keller (NIST), aims to develop phase field benchmark problems for the global phase field community. To date, four CHiMaD Phase field workshops have been organized to engage the community for their input in developing the benchmark problems. A website has been developed by Wheeler (NIST) as a part of this collaboration *(https://pages.nist.gov/chimad-phase-field/#benchmarks)*. This initiative has also resulted in a publication in *Computational Materials Science* [25.30], which has been selected as the Editor's Choice.

Phase Field Method Development

*Peter **Voorhees** (NU), James **Warren** (NIST)*

Together with Ofori-Opoku (NIST), **Voorhees** (NU) and **Warren** (NIST) are developing the phase field crystal method for faceted interfaces.

11.2.3 External Collaborations

Scalable Computational Models and Codes

*Olle **Heinonen** (ANL), Serge Nakhmanson (University of Connecticut)*
Through this collaboration scalable computational models and codes for coupled ferroelectric-elastic systems are being developed.

Phase Field Methods

*Peter **Voorhees** (NU), Henning Poulsen (Techical University of Denmark)*
Through this collaboration a formalism was introduced for quantitative comparisons between volumetric time-resolved experimental and simulated data, based on measurements of the position of microstructural interfaces. The formalism presents a method to determine material parameters by finding the value of simulation parameters producing the best match between experiment and simulation by variation. The results of collaboration has been accepted for publication in *Acta Materiala* [25.31].

11.3 Technology Transfer

Community Resource

CHiMaD Phase Field Website

*D. Wheeler (NIST), Olle **Heinonen** (ANL), Peter **Voorhees** (NU), James **Warren** (NIST), Jonathan **Guyer** (NIST)*
Link: https://pages.nist.gov/chimad-phase-field
CHiMaD Phase Field Website is a resource for the phase field community to compare and contrast phase field codes and libraries with an aim to improve community code collaboration. The first set of benchmark problems for phase field methods, which grew out of the CHiMaD Phase Field workshops I-III and constructed with feedback from the workshops was published in *Computational Materials Science* as an Editor's Choice publication [25.30]. The benchmark problems, together with one set of solutions, are posted on the CHiMaD Phase Field Website. It is expected that these benchmark problems will be a significant resource for developers of phase field codes - the problems are already being used in college courses taught by CHiMaD Phase Field Methods workshop contributors such as by Mike Tonks (Penn State). A second set of benchmark problems are in preparation and will be tested during the workshops organized in 2017.

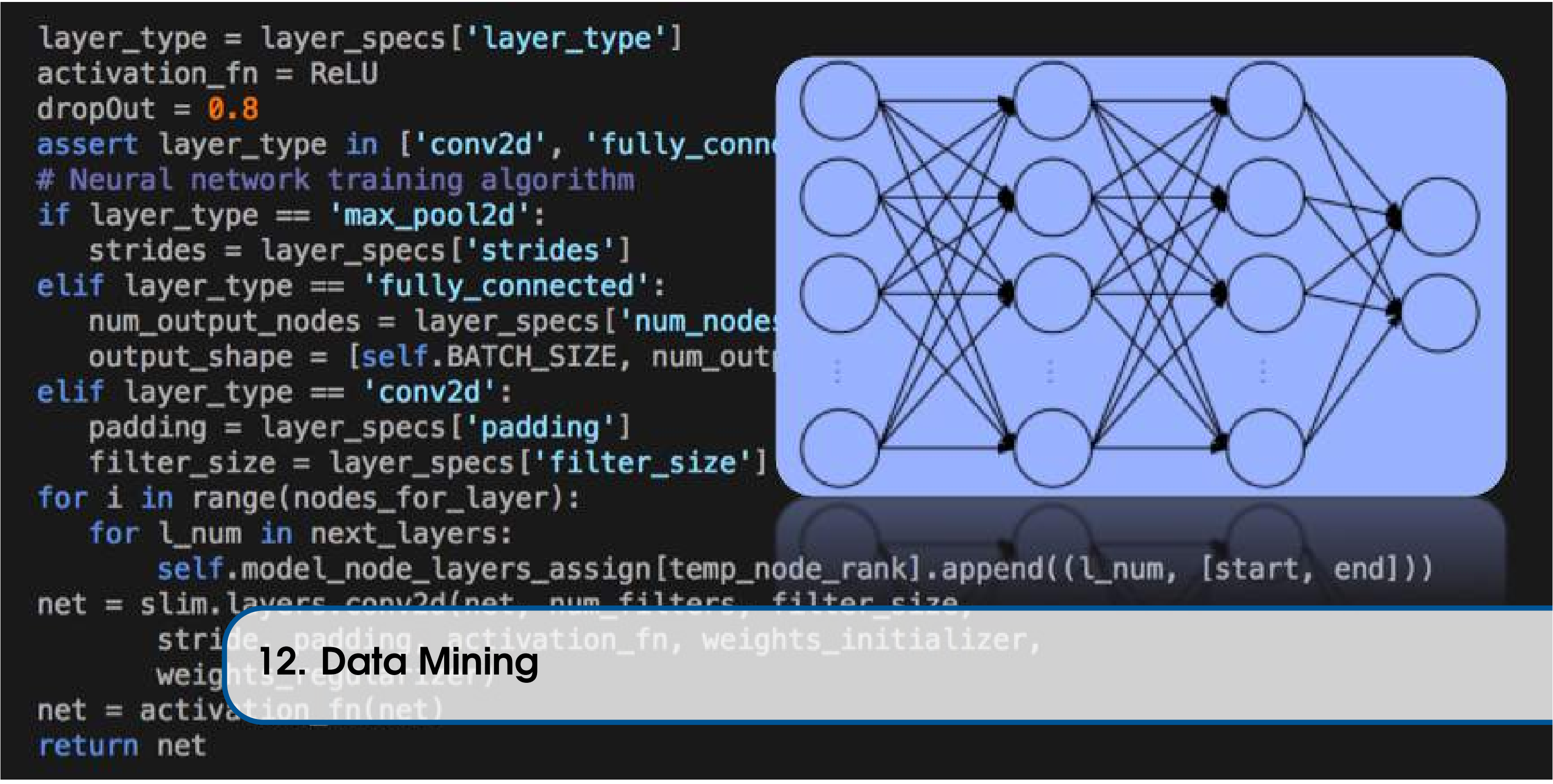
11.4 Publications and Presentations

4 Number of CHiMaD-supported publications in 2016 by Phase Field Methods seed group. Please see chapter 25 for details [25.26, 25.29, 25.30, 25.31].

8 Number of presentations on CHiMaD supported research in 2016, please see section 24.9 for the complete list.

11.5 CHiMaD Team

Phase Field Methods Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Olle Heinonen Peter Voorhees David Chopp Barry Smith	Principal Investigator Principal Investigator Principal Investigator Principal Investigator	ANL/NAISE NU/MSE NU/ESAM ANL/NAISE	
Nana Ofori-Opoku	Postdoctoral Researcher	NU/NIST	Phase Field Crystal Methods for Facetted Interfaces *(Voorhees/Warren)*
Andrea Jokisaari	Postdoctoral Researcher	NU/NAISE	Phase field benchmark problems *(Heinonen/Smith)*
Stefan Poulsen	Postdoctoral Researcher	NU/MSE	Methods for Determining Difficult to Measure Materials Properties *(Voorhees)*
Narut Sereewattanawoot	Graduate Student	NU/ESAM	PLATS Methodology *(Chopp)*



```
layer_type = layer_specs['layer_type']
activation_fn = ReLU
dropOut = 0.8
assert layer_type in ['conv2d', 'fully_conn
# Neural network training algorithm
if layer_type == 'max_pool2d':
   strides = layer_specs['strides']
elif layer_type == 'fully_connected':
   num_output_nodes = layer_specs['num_node
   output_shape = [self.BATCH_SIZE, num_out
elif layer_type == 'conv2d':
   padding = layer_specs['padding']
   filter_size = layer_specs['filter_size']
for i in range(nodes_for_layer):
   for l_num in next_layers:
       self.model_node_layers_assign[temp_node_rank].append((l_num, [start, end]))
net = slim.layers.conv2d(net, num_filters, filter_size,
       stride, padding, activation_fn, weights_initializer,
       weights_regularizer)
net = activation_fn(net)
return net
```

12. Data Mining

Alok Choudhary (NU), Ankit Agrawal (NU), Gregory Olson (NU), Chris Wolverton (NU), Wei Chen (NU), Peter Voorhees (NU)

Carelyn Campbell (NIST), Alden Dima (NIST), Martin Green (NIST), Gilad Kusne (NIST), Sheng Yen Li (NIST)

Significance

The CHiMaD data mining team is working towards making significant advances in data-driven informatics to accelerate materials discovery. In this era of big data, we are being bombarded with huge volumes of data from a variety of different sources (experiments, simulations) at unprecedented rates in practically all fields of science and engineering, and materials science is no exception. Advanced techniques for data-driven analytics are needed to analyze all this data in ways that can help extract meaningful information and knowledge from it, and thus contribute to accelerating materials discovery and the vision of Materials Genome Initiative. The diversity and expertise within the CHiMaD team provides unique opportunities for collaborations among materials scientists and computer scientists to realize this goal. This requires designing and developing specific analytics and data mining approaches for problems in materials science, and evaluating the resulting insights/discoveries via necessary experiments and simulations. The long-term vision is to work with NIST to enable data-to-discovery (or actionable insights) at unprecedented latency through summary statistics, query, reporting, analysis, bottom-up as well as hypothesis-driven discoveries and data mining on various heterogeneous and big databases that are complex, high dimensional, structured and semi-structured.

12.1 Design Goals

The design goals of the Data Mining use-case group for this reporting period were four-fold:

- Continue to make progress in the ongoing collaborative materials informatics projects from prior years

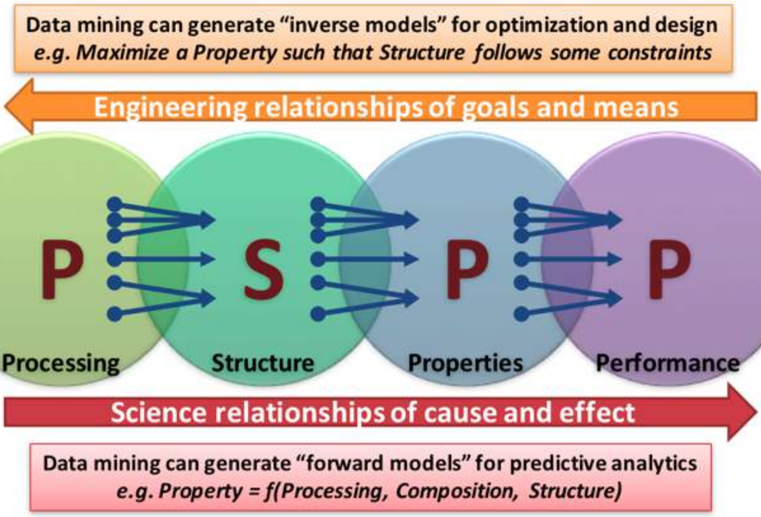


Figure 12.1: The processing-structure-property-performance relationships of materials science and engineering, where the deductive science relationships of cause and effect flow from left to right, and the inductive engineering relationships of goals and means flow from right to left. Further, it is important to note that each relationship from left to right is many-to-one, and consequently the ones from right to left are one-to-many. Data mining approaches can help decipher these relationships via forward and inverse models.

- Design and develop software deploying materials informatics for the materials community to use
- Make efforts towards validating the predictions from our data mining models via experiments
- Explore new projects and collaborations to solve important problems in materials science that can benefit from data-driven informatics

The ongoing projects of the Data Mining tool group includes efforts towards mining the Open Quantum Materials Database (OQMD), Japan National Institute for Materials Science (NIMS) MatNavi steel database, microstructure characterization and reconstruction, and integrating CALPHAD and data mining for advanced steel design in support of the precipitation-strengthened alloys use-case group. Further, some user-friendly online tools for predicting properties of a given material developed and released, which can essentially serve as fast proxies for experiments or simulations to understand the science of materials (forward models of PSPP relationships, as depicted in Figure 12.1), and in turn also aid in the engineering and design of materials with desired properties (inverse models of PSPP relationships). This year Data Mining tool group researchers have also validated some of our prior data mining predictions of glass forming ability in a ternary system with the help of an external collaboration with experimentalists. A few new efforts have been initiated this year towards investigating the use of data-driven methodologies for predicting properties of thermoelectric materials, organic photovoltaics, and search for quaternary Heusler compounds. Finally, new collaborative projects have been initiated with NIST researchers on using data mining to discover improved Ni-Al-Cr superalloys, and classifying x-ray diffraction images.

12.2 Significant Accomplishments in 2016

Following are the significant accomplishments of the data mining team in the past year:

- In collaboration with **Choudhary** (NU), **Wolverton** (NU), and Meredig (NU), **Agrawal** (NU) has developed an online tool deploying machine learning models to predict formation energy of a set of chemical compositions.
- In collaboration with **Agrawal** (NU), **Choudhary** (NU), and **Wolverton** (NU), graduate student Ward (NU) has developed a general-purpose machine learning framework for predicting properties of inorganic materials.
- In collaboration with **Agrawal** (NU), **Choudhary** (NU), **Wolverton** (NU), graduate students Ward (NU), Liu (NU), Krishna (NU), and Hegde (NU) have developed a structure-aware data mining model to predict formation energy for a chemical compound with a given crystal structure.
- In collaboration with **Agrawal** (NU), **Choudhary** (NU), and **Wolverton** (NU), graduate students Liu (NU), Jha (NU) and Ward (NU) have developed the most accurate models for predicting formation energy till date using deep learning.
- In collaboration with **Choudhary** (NU), **Agrawal** (NU) has developed an online tool deploying machine learning models to predict the fatigue strength of steel alloys based on their composition and processing parameters.
- In collaboration with **Chen** (NU) and Apley (NU), doctoral student Bostanabad (NU) has developed a supervised learning based microstructure characterization and reconstruction approach for 2D and 3D microstructures.
- In collaboration with **Agrawal** (NU) and **Choudhary** (NU), research associate Furmanchuk (NU) has developed predictive models for bulk modulus of crystalline materials.
- In collaboration with **Agrawal** (NU), **Choudhary** (NU), Voorhees, **Wolverton** (NU), graduate students Kim (NU), Krishna (NU), and Ward (NU) have developed a machine learning model using data from the OQMD to predict new Quaternary Heusler compounds.
- A collaboration between *Liquidmetal Technologies* and **Wolverton** (NU) group showed that it is possible to tailor the properties of commercial metallic glasses alloys with guidance from machine learning models.
- A collaboration between **Wolverton** (NU) group and researchers at University of South Carolina and the SLAC National Accelerator Laboratory discovered new metallic glasses in a ternary system with high-throughput experimentation, validating our prior prediction.
- In collaboration with **Agrawal** (NU), **Choudhary** (NU), and research associate Furmanchuk (NU), graduate student Paul (NU) has developed predictive models for OPV properties using molecular fingerprints.
- A team of undergraduates in special Murphy Scholar section of Freshman Design Thinking and Communications course at NU collaborated with **Agrawal** (NU), **Choudhary** (NU), **Olson** (NU), former research associate Xiong (UPitt), and QuesTek materials engineer Saboo (QuesTek) to augment the NIMS database with thermodynamic parameters calculated using CALPHAD-driven models.

12.3 Research Accomplishments

A Formation Energy Predictor for Crystalline Materials Using Ensemble Data Mining

This collaborative project between **Agrawal** (NU), **Choudhary** (NU), **Wolverton** (NU)

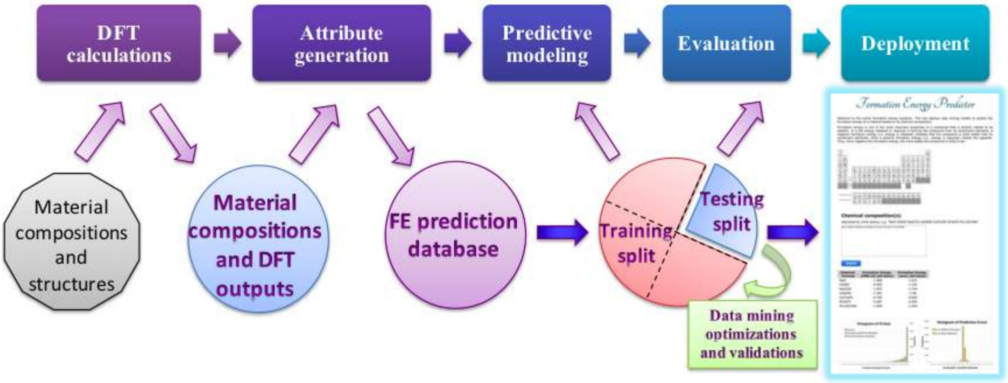


Figure 12.2: The design of the data mining workflow used to build formation energy prediction models. DFT calculations on hundreds of thousands of compounds have been done and stored in OQMD. Only composition information was used to derive additional attributes and build ensemble predictive models. The most accurate models were deployed in the online formation energy predictor tool.

and former graduate student Meredig (NU) has developed and deployed accurate predictive models for formation energy using ensemble data mining methodologies, using only the chemical composition of the material. These data-driven models were built using hundreds of thousands of Density Functional Theory (DFT) calculations, which is a quantum mechanical simulation technique based on the electron density within the crystal structure of the material. These models were deployed in an online web-tool that takes a list of material compositions as input, generates over hundred composition-based attributes for each material and feeds them into the predictive models to obtain the predictions of formation energy, and thus convert a set of compositions to a ranked list in the order of predicted stability (Figure 12.2). Such a tool with fast and accurate predictive models of formation energy can be used to screen a list of chemical compositions and subsequently use that information to guide experiments and simulations. The online formation energy predictor is available at *http://info.eecs.northwestern.edu/FEpredictor*. This work has been published as a demonstration paper in the *Proceedings of IEEE International Conference on Data Mining (ICDM 2016)* [25.39].

A General-Purpose Machine Learning Framework for Predicting Properties of Inorganic Materials In collaboration with **Agrawal** (NU), **Choudhary** (NU), **Wolverton** (NU), graduate student Ward (NU) has created an extensive set of composition-based parameters of materials (including and beyond the ones used in our prior work) that could be coupled with data mining to effectively predict a wide variety of material properties. This new method drastically simplifies the construction of machine learning models for materials properties, which will enable faster development of these useful models for many different materials engineering challenges. What is particularly exciting is that this method can create accurate models for applications as different as crystalline solar cells and amorphous metal alloys without any problem-specific modifications. As shown in Figure 12.3, a machine learning model trained without any data from the Al-Ni-Zr ternary system could accurately predict the existence, locations, and relative sizes of the two glass-forming regions. This work has been published in *npj Computational Materials* [25.41].

Fast and accurate models for formation energy of crystalline compounds using Voronoi tessellations and machine learning This is a collaborative work between **Agrawal** (NU),

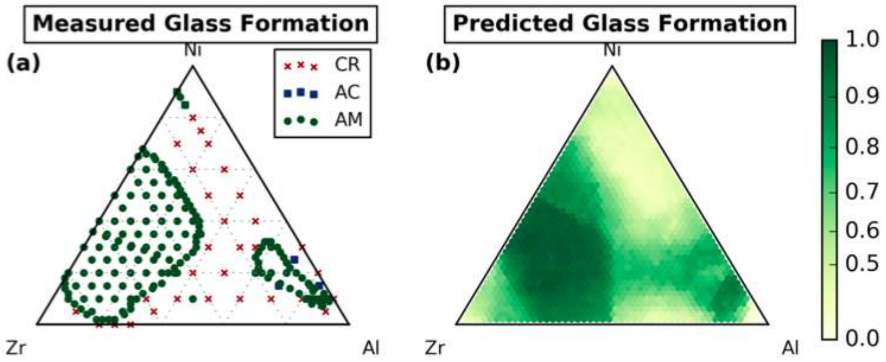


Figure 12.3: (Left) Experimentally-measured regions of glass-forming ability in the Al-Ni-Zr ternary system. (Right) Predicted glass-forming ability by a machine learning model that was trained without any data from the diagram present on the left

Choudhary (NU), **Wolverton** (NU), and graduate students Ward (NU), Liu (NU), Krishna (NU), and Hegde (NU), where the goal is to go a step further and add crystal structure information into the data mining model. In addition to the composition-based attributes used in our prior work, this technique involves the use of additional length-scale-independent attributes derived from Voronoi tessellation of the compound's crystal structure. ML models created using this method have half the cross-validation error and similar computation times to models created with the Coulomb matrix and Pair Radial Distribution Function (PRDF) methods (see Figure 12.4). A manuscript based on this work is in preparation.

Deep Learning for Chemical Compound Stability Prediction Deep learning is a recent revolutionary breakthrough in machine learning, arisen from a rediscovery of deep neural networks, and fueled by the availability of two key ingredients - big data and big compute - that are becoming increasingly available and affordable over the past few years. The way in which the data is represented can make a huge difference in the success of a learning algorithm, and deep learning enables the learning of multiple levels of representation, by discovering more abstract features at higher levels. It is considered a very powerful method to build large-scale recognition systems to exploit the information locked in big data. Deep learning has enabled ground-breaking achievements in various fields, such as computer vision, speech recognition, etc., and as part of the CHiMaD project, we envision to leverage these advances and develop deep learning driven solutions for materials property prediction, materials discovery, and materials design.

We have already started exploring this direction in some of the projects, and have got some encouraging results. A collaboration between **Agrawal** (NU), **Choudhary** (NU), **Wolverton** (NU), graduate students Liu (NU), Jha (NU) and Ward (NU), and research professor Wei-keng Liao (NU) investigated the efficacy of deep learning models on the Open Quantum Materials Database (OQMD) to predict the chemical compound stability, using *only* elemental fractions as the input (see Figure 12.5), rather than including hundreds of hand-engineered attributes. This is expected to provide an end-to-end modeling from atom fractions to materials property (in this case, formation energy), and improve model interpretability and usability for non-domain experts. In our experiments on over 300,000 compounds from OQMD, a seven-layered deep neural network with dropouts and probabilistic initialization of neural-network weights was found to result in the best model (formation energy prediction MAE of 0.072 eV/atom), which is significantly better than

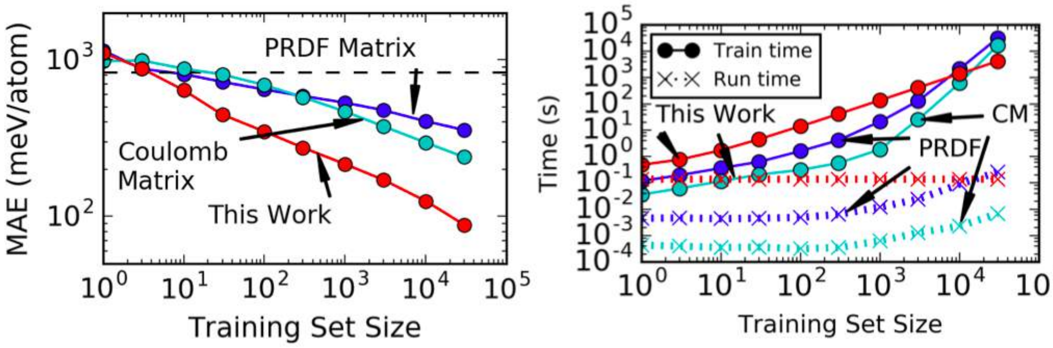
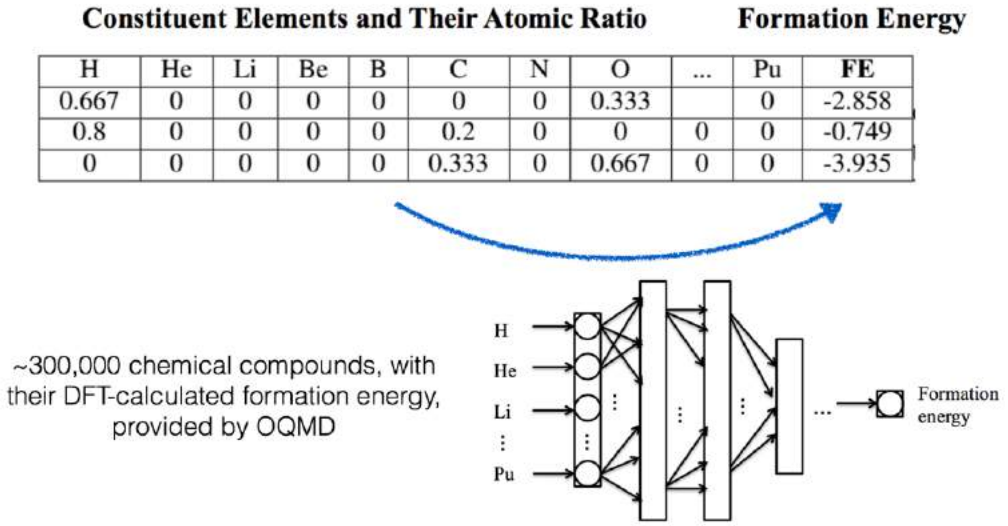


Figure 12.4: (Left) Mean absolute error (MAE) measured using cross-validation of models created using the PRDF Matrix *[Phys. Rev. B 89, 205118 (2014)], Coulomb Matrix [Int. J. Quantum Chem. 115, 1094 (2015)]* and our proposed method. Each model was trained on the DFT formation energies of a set of randomly-selected compounds from the ICSD and used to evaluate 1000 distinct compounds that were also selected at random. The black, dashed line indicates the expected error from guessing the mean formation energy of the training set for all structures. (Right) Comparison of model training and running time of the three methods to predict the formation energy of inorganic compounds. Training time is the sum of attribute generation and model construction with given data. Run time is the average time taken to compute the required attributes and evaluate the machine learning model for a single compound.


Constituent Elements and Their Atomic Ratio **Formation Energy**

H	He	Li	Be	B	C	N	O	...	Pu	**FE**
0.667	0	0	0	0	0	0	0.333		0	-2.858
0.8	0	0	0	0	0.2	0	0	0	0	-0.749
0	0	0	0	0	0.333	0	0.667	0	0	-3.935

Figure 12.5: Schematic for deep learning system. The training algorithm learns the relationship between the input elemental fractions and output formation energy via multiple hidden layers of neurons, without any additional hand-engineered attributes.

Steel Fatigue Strength Predictor

Welcome to the steel fatigue strength predictor. This tool is built using experimental data of more than 400 steels, available from the Japan National Institute for Materials Science (NIMS) MatNavi database. This database consists of processing and composition information of steels, along with the experimentally measured rotating bending fatigue strength (10 million cycles). Various data analytics techniques such as feature selection and regression modeling were used to obtain highly accurate fatigue strength prediction models using a small non-redundant set of six composition parameters and three processing parameters.

The tool estimates the fatigue strength of the steel based on the composition and processing parameters entered by the user. To obtain the fatigue strength prediction, please enter the attribute values below, and click the submit button.

Carbon (C) (wt %) 0.388
Silicon (Si) (wt %) 0.3
Phosphorus (P) (wt %) 0.016
Chromium (Cr) (wt %) 0.57
Copper (Cu) (wt %) 0.068
Molybdenum (Mo) (wt %) 0.07
Through Hardening Temperature (°C) 850
Cooling Rate for Through Hardening (°C/hr) 8
Tempering Time (minutes) 60

Have more attributes to enter?

Use the full calculator instead!

Predicted fatigue strength of the given steel = **512.788 MPa**

Figure 12.6: (Top-left) Data-driven methodology used to build the steel fatigue strength predictor. (Bottom-left) Illustrative results demonstrating that the new ensemble models outperform the prior best models, especially in the low fatigue strength region where the old model had failed. (Right) A screenshot of the deployed steel fatigue strength predictor.

the models built using traditional machine learning techniques. At the same time, these models run about an order of magnitude faster than other machine learning models. This enhanced performance comes at the cost of increased training time though, although it is just a one-time cost to build the model. Preliminary results from this work were presented at the *ACM SIGKDD workshop on Large-Scale Deep Learning for Data Mining (DL-KDD 2016)* [25.43].

A Fatigue Strength Predictor of Steels Using Ensemble Data Mining In this project, **Agrawal** (NU) and **Choudhary** (NU) have developed accurate forward predictive models for steel fatigue strength using a publicly available dataset from Japan National Institute of Materials Science (NIMS) MatNavi database. The models are build using advanced data-driven ensemble predictive mining techniques and possess an extremely high cross-validated accuracy of >98%. We have also deployed these models in a user-friendly online web-tool, which can make very fast predictions of fatigue strength for a given steel represented by its composition and processing information (see Figure 12.6). Such a tool with fast and accurate models is expected to be a very useful resource for the materials science researchers and practitioners to assist in their search for new and improved quality steels. The web-tool is available at *http://info.eecs.northwestern.edu/SteelFatigueStrengthPredictor*. This work has been published as a demonstration paper in the proceedings of *ACM International Conference on Information and Knowledge Management (CIKM 2016)* [25.38].

Characterization and Reconstruction of 3D Stochastic Microstructures via Supervised Learning In collaboration with **Chen** (NU) and Apley (IEMS department, NU), graduate student Bostanabad (NU) has developed a supervised learning based microstructure characterization and reconstruction approach for both 2D and 3D microstructures. The methodology is general in that it can be applied to a broad range of microstructures (clustered, porous, and anisotropic). By treating the digitized microstructure image as a set of training data, it generically learns the stochastic nature of the microstructure via fitting a supervised learning model to it using classification trees. The fitted supervised learning

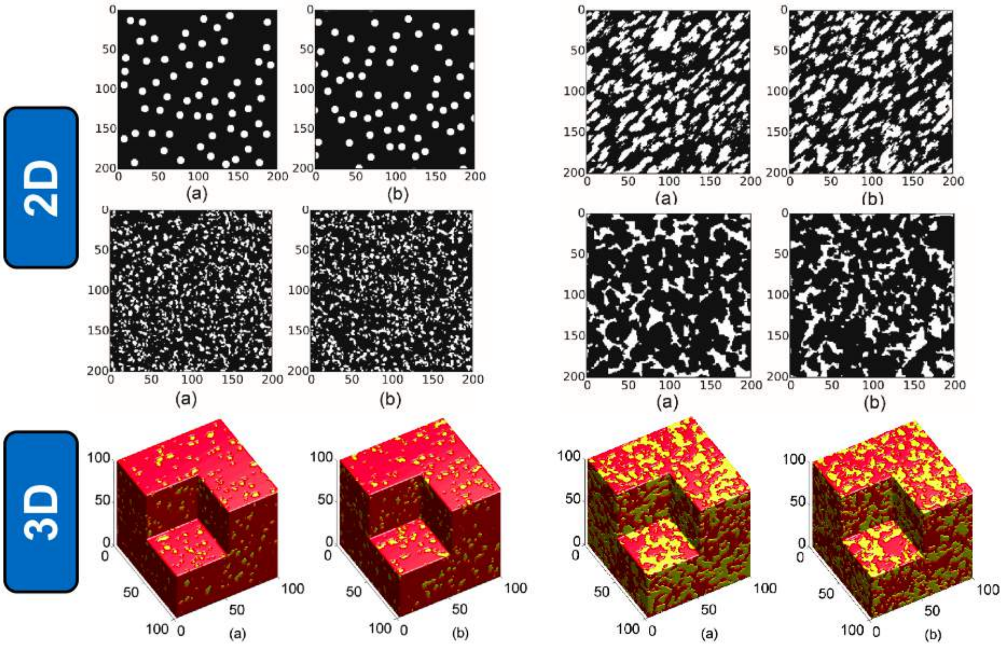


Figure 12.7: Reconstruction through Supervised Learning: Reconstructed images in (b) are statistically equivalent to the original images in (a). The method is shown to be effective for a broad range of microstructures.

model provides an implicit characterization of the joint distribution of the collection of pixel phases in the image. The approach has been validated on a variety of material systems and it has been demonstrated to be computationally efficient in reconstructing 3D microstructures (see Figure 12.7). This work has been published in the *Journal of Microscopy* [25.44].

Predictive analytics for thermoelectric materials In collaboration with **Agrawal** (NU) and **Choudhary** (NU), research associate Furmanchuk (NU) has developed predictive models for bulk modulus of crystalline materials, supported primarily by the DARPA SIMPLEX project on data-driven discovery for designed thermoelectric materials, and partially by the NIST CHiMaD project. The bulk modulus is one of the important parameters for designing advanced high-performance and thermoelectric materials. This work represents the first attempt to develop a generalized model for forecasting bulk modulus of various types of crystalline materials, based on ensemble predictive learning using a unique set of attributes. The attributes used are a combination of experimentally measured structural details of the material and chemical/physical properties of atoms. The model was trained on a data set of stoichiometric compounds calculated using density functional theory (DFT). It showed good predictive performance when tested against external DFT-calculated and experimentally measured stoichiometric and non-stoichiometric materials. The generalized model found correlations between bulk modulus and features defining bulk modulus in specific families of materials. This work has been published in *RSC Advances* [25.40].

Accelerated Search for New Quaternary Heusler Compounds This collaboration project between **Agrawal** (NU), **Choudhary** (NU), **Voorhees** (NU), **Wolverton** (NU), and graduate students Kim (NU), Krishna (NU), and Ward (NU), initiated as PSED project and is being continued under partial CHiMaD support (PSED is the Predictive Science & Engineering Design doctoral cluster program at Northwestern co-directed by **Chen**, **Olson**, and **Liu**). This project uses machine learning and data from the OQMD to predict new Quaternary Heusler compounds. Quaternary Heuslers are a class of crystalline compounds that share the same order arrangement of four elements on a body-centered cubic lattice, and have been found to exhibit many intriguing properties. However, finding new Quaternary Heuslers is difficult. Out of the nearly 100,000 candidate Heuslers that the **Wolverton** (NU) group has evaluated with DFT to date, fewer than 1% were found to be stable. To more efficiently search the remaining 2.9 M Heusler compounds, we constructed a machine learning model based on data from the OQMD and the Voronoi-tessellation-based technique we developed last year. With this model, around two dozen stable Heuslers were found with only a few hundred additional DFT calculations - a success rate an order of magnitude higher than the original search!

Improved Properties of Commercial Metallic Glasses Alloys with Machine Learning As part of a collaboration with *Liquidmetal Technologies* and **Wolverton** (NU) group, machine learning models to predict two key processing properties of metallic glasses were constructed: the critical casting thickness and temperature range of the supercooled liquid. These models were constructed based on data from the scientific literature and the "general-purpose" attribute set we have developed previously. These models were employed to find small adjustments to the composition of commercial alloys that optimize both of the target properties. Some of the predicted alloys exceeded both base alloys in the size of the supercooled liquid range at only a slight degradation of casting thickness. These results demonstrate how it is possible to tailor the properties of metal alloys with guidance from machine learning models.

Discovery of New Ternary Metallic Glasses with High-Throughput Experimentation Using a machine-learning model trained on the results on thousands of melt-spinning and sputtering experiments, the data mining group researchers had previously predicted that it is possible to form metallic glasses in the Co-V-Zr ternary system. Recently, in a collaboration between the **Wolverton** (NU) group and researchers at University of South Carolina and the SLAC National Accelerator Laboratory, this prediction was confirmed. Using a combination of co-deposition and high-throughput X-ray diffraction analysis, our collaborators sampled the glass-forming ability of hundreds of compositions in this ternary and identified a broad range of alloys that can form metallic glasses. This experimental information can be fed back into the machine learning models to make even more accurate predictions of other candidate alloys.

Organic Photovoltaics Data Mining In collaboration with **Agrawal** (NU), **Choudhary** (NU) and research associate Furmanchuk (NU), graduate student Paul (NU) has been developing a model for predicting the properties of OPVs (specifically highest occupied molecular orbital (HOMO) in the donor layer) using molecular fingerprints by employing ensemble and regularized regression methods on the Harvard Organic Photovoltaic (HOPV) dataset. This is an ongoing collaboration between the Data Mining and OPV groups.

Integrating CALPHAD and data mining for advanced steel design (precipitation- strengthened alloys use-case) This collaboration between **Agrawal** (NU), **Choudhary** (NU), **Olson** (NU), former research associate Xiong (UPitt), and Saboo (QuesTek), aims to design an effective interface between data mining and CALPHAD methodology for materials genomic design of advanced steels. This project utilizes carbon steels fatigue strength data, with raw data sets obtained from experiments provided by NIMS Japan. The means to integrate CALPHAD and data mining in this project is to use CALPHAD to enrich steel composition and processing data with structure information to derive more reliable data-driven structure-property linkages via data mining. Building upon the data mining efforts in prior years along this direction, a team of undergraduates in special Murphy Scholar section of Freshman Design Thinking and Communications course (NU) collaborated with data mining team to compute thermodynamic parameters for the steels in the NIMS database. In particular, more accurate values for martensite-start temperature, austenite stability parameter, and retained austenite fraction were calculated, as these were found to be the three most important thermodynamic parameters influencing the fatigue strength by our earlier data mining analysis. Our team is continuing to work along these lines after the completion of the undergraduate project.

12.4 Collaborations

12.4.1 CHiMaD Collaborations

Large Scale Data-driven analytics of quantum mechanical calculations (DFT data mining)
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Christopher **Wolverton** (NU)*
This collaboration is geared towards applying data mining techniques for predictive modeling of various materials properties using the Open Quantum Materials Database (OQMD). It involves several projects using different types of materials representations and advanced data-driven methods for materials property prediction.

Steel fatigue data mining using processing and composition information
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU)*
This project developed accurate forward predictive models for steel fatigue strength using a publicly available dataset, and also released an online software tool for the same.

Integrating CALPHAD and data mining for advanced steel design
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Gregory **Olson** (NU)*
This collaboration aims to use CALPHAD to enrich steel composition and processing data with structure information to derive more reliable data-driven structure-property linkages.

Accelerated Search for New Quaternary Heusler Compounds
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Peter **Voorhees** (NU), Christopher **Wolverton** (NU)*
This project uses machine learning and data from the OQMD to predict new Quaternary Heusler compounds. This collaboration began as a PSED project.

Constructing Precipitate Growth Models with Machine Learning
*Christopher **Wolverton** (NU), Gregory **Olson** (NU)*
This collaboration employing machine learning models to predict the size of precipitates in aluminum alloys as a function of alloy composition and aging conditions.

OPV data mining
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU)*
This project aims at developing predictive models for highest occupied molecular orbital (HOMO) of the donor layer for organic photovoltaics (OPVs).

Thermoelectrics data mining
*Ankit **Agrawal** (NU), Alok **Choudhary** (NU), Gregory **Olson** (NU)*
This project aims at developing predictive models for thermoelectric properties of compounds and materials, and is primarily supported by the DARPA SIMPLEX project and managed by NAISE/CHiMaD.

12.4.2 NIST Collaborations

Classification of Scientific Journal Articles to Support NIST Data Curation Efforts

Ankit ***Agrawal*** *(NU), Alok* ***Choudhary*** *(NU), Alden* ***Dima*** *(NIST), Kenneth* ***Kroenlein*** *(NIST), Sarala* ***Padi*** *(NIST), Adele* ***Peskin*** *(NIST)*

This collaboration is aimed at supporting the data curation effort of the NIST Thermodynamic Research Center (TRC) by classifying an article as relevant or not relevant to their data extraction pipeline. An online tool deploying the classifier is under construction (beta version available at: http://info.eecs.northwestern.edu/TRCArticleClassifier)

Data-driven design of Ni-Al-Cr superalloy

Ankit ***Agrawal*** *(NU), Alok* ***Choudhary*** *(NU), Carelyn* ***Campbell*** *(NIST), Sheng Yen* ***Li*** *(NIST)*

This is a new collaboration that aims at using data-driven techniques to predict work-to-necking of a given Ni superalloy, and subsequently discover new superalloys with optimal desired properties.

X-ray diffraction image classification

Gilad ***Kusne*** *(NIST), Martin* ***Green*** *(NIST), Ankit* ***Agrawal*** *(NU), Alok* ***Choudhary*** *(NU)*

This is a new collaboration that aims at using data-driven techniques to classify x-ray diffraction images into structure classes.

12.4.3 External Collaborations

Structural Equation Modeling

Wei ***Chen*** *(NU), Dan Apley (NU/Department of Industrial Engineering and Management Science)*

Through this collaboration, **Chen** and Apley (NU)are developing the supervised based learning algorithm for microstructure characterization and reconstruction.

Engineering and Discovering Bulk Metallic Glass Alloys with Machine Learning

Christopher ***Wolverton*** *(NU), Liquidmetal Technologies*

Liquidmetal Technologies is a world leader in commercial bulk metallic glass alloys. **Wolverton** (NU) groups leads the optimization existing commercial alloys for two processability related properties with machine learning models, in collaboration with researchers at *Liquidmetal Technologies*.

High-Throughput Experimental Search for New Amorphous Metal Alloys

Christopher ***Wolverton*** *(NU), Jason Hattrick-Simpers (U. South Carolina), Apurva Mehta (SLAC)*

In collaboration with groups specializing in combinatorial experimentation and high-throughput x-ray characterization, **Wolverton** (NU) group discovered a range of new metallic glasses that were originally predicted by a machine learning model.

Active Learning for the Faster Discovery of Bulk Metallic Glasses

Christopher ***Wolverton*** *(NU), Katharine Flores, Roman Garnett (Washington U.)*

This collaboration is designed to lay the groundwork for an automated system for discovering new bulk metallic glass alloys: the development of an approach that will automatically determine the fewest number of experiments necessary to create an accurate model for glass-forming ability and identify new amorphous alloys.

Data Analytics for Understanding and Predicting New Perovskite Materials

Christopher ***Wolverton*** *(NU), Turab Lookman (Los Alamos National Laboratory)*

Researchers at LANL have assembled a dataset of the compositions of all known ABO_3 oxide materials. **Wolverton** (NU) group are working with them to build improved machine learning models with this database, and use them to develop techniques to predict the compositions of new perovskite materials.

12.5 Technology Transfer

Software
Steel Fatigue Strength Predictor
A. Agrawal, A. Choudhary
Date: 10/26/16
Distribution: Public
Access Link: http://info.eecs.northwestern.edu/SteelFatigueStrengthPredictor
This online software tool estimates the fatigue strength of the steel based on the composition and processing parameters entered by the user. The predictive models deployed in this tool were built on publicly available data. All the models and software for the online tool have been developed by **Agrawal** (NU). This tool was presented at a major computer science conference (CIKM) in 2016, and shall also be demonstrated at TMS in 2017.

Software
Formation Energy Predictor
A. Agrawal, B. Meredig, C. Wolverton, A. Choudhary
Date: 12/13/16
Distribution: Public
Access Link: http://info.eecs.northwestern.edu/FEpredictor
This is an online software tool predicts the formation energy of a material based on its chemical composition. The predictive models deployed in this tool were built using DFT data from OQMD. Several models are deployed in this tool, and we shall continue to add new advanced predictive models to this tool as we develop them. Currently available models and software for the online tool were developed by **Agrawal** (NU). This tool was presented at one of the top data mining conference (ICDM) this year.

Software
Versatile Atomic Scale Structural Analysis Library (Vassal)
L. Ward, C. Wolverton
Distribution: Private
Access Link: http://bitbucket.org/wolverton/vassal
Vassal is a software library designed to support the creation of machine learning models from atomic-scale structure data. It includes methods necessary to replicate many common structural analysis techniques employed in the literature, and is designed to easily interface with our group's materials analytics software, Magpie.

12.6 Publications and Presentations

10 Number of CHiMaD-supported publications in 2016 by Data Mining Tool group. Please see chapter 25 for details [25.37, 25.38, 25.39, 25.40, 25.41, 25.42, 25.43, 25.44, 25.45, 25.46].

40 Number of presentations on CHiMaD supported research in 2016, please see section 24.12 for the complete list.

12.7 CHiMaD Team

Data Mining Use-Case Group Researchers			
Name	**Position**	**Affiliation**	**Project (PI)**
Alok Choudhary Ankit Agrawal Gregory Olson Christopher Wolverton Wei Chen	Principal Investigator Principal Investigator Principal Investigator Principal Investigator Principal Investigator	NU/EECS NU/EECS NU/MSE NU/MSE NU/ME	
Wei-keng Liao	Research Faculty	NU/EECS	DFT data mining *(Choudhary, Agrawal)*
Wei Xiong	Research Associate	NU/MSE	CALPHAD Databases *(Olson)*
Al'ona Furmanchuk	Research Associate	NU/EECS	Thermoelectrics data mining *(Choudhary, Agrawal)*
Amar Krishna	Graduate Student	NU/EECS	DFT data mining, NIST TRC article classification *(Choudhary, Agrawal)*
Rouqian Liu	Graduate Student	NU/EECS	DFT data mining *(Choudhary, Agrawal)*
Arindam Paul	Graduate Student	NU/EECS	OPV data mining *(Choudhary, Agrawal)*
Dipendra Kumar Jha	Graduate Student	NU/EECS	DFT data mining *(Choudhary, Agrawal)*
Logan Ward	Graduate Student	NU/MSE	Machine Learning for Materials Discovery *(Wolverton)*
Xiaochen Ren	Graduate Student	NU/ME	Substitutional doping and alloy formation in transition metal dichalcogenides *(Chen)*
Yichi Zhang	Graduate Student	NU/ME	Microstructure Characterization and Reconstruction *(Chen- external funding)*
Ramin Bostanabad	Graduate Student	NU/ME	Microstructure Characterization and Reconstruction *(Chen- external funding)*
Xiaolin Li	Graduate Student	NU/ME	Microstructure Characterization and Reconstruction *(Chen/Brinson- external funding)*

13. Metals Processing Facility

Manager: Paul Adler (NU)
1801 Maple Avenue, Evanston, IL, USA 60201

Significance

The paradigm of computational design of material systems has been shown to significantly reduce time from ideation to component qualification. Despite the advantage of rapid prototyping via virtual simulation some experimentation is still required for model refinement. Initial testing typically involves production of buttons of desired composition mainly to verify predicted phase fractions, chemical partitioning, and cast microstructures. Scale-up manufacture of designed alloys will involve processing effects that greatly influence the final microstructural and thus property gradients. The goal of this effort is to construct a metal processing laboratory capable of capturing these effects for the expressed purpose of further refinement of computational models of promising systems.

13.1 Metals Processing Facility

The CHiMaD Metals Processing Facility construction was completed on March 18, 2016, Figure 13.1. The first piece of equipment to be moved in was the Buehler AM/0.5 Arc Melter; it is currently operational and in-use, Figure 13.2. Two large pieces of equipment, the Torrington 100 and 211 Swagers and Fenn 2/4 Hi Rolling Mill are currently out for refurbishing. A before and after photo of the Rolling Mill is shown in Figure 13.3

Currently Available Equipment

- Buehler AM/0.5 Arc Melter
- Torrington 100 and 211 Swagers - currently being refurbished, Torrington 100 will be replaced by a rebuilt Fenn 4F-4 unit
- Fenn 2/4 Hi Rolling Mill - currently being refurbished, Figure 13.3
- Limit Dome Height Testing Unit
- HPM 150 ton Hydraulic Press

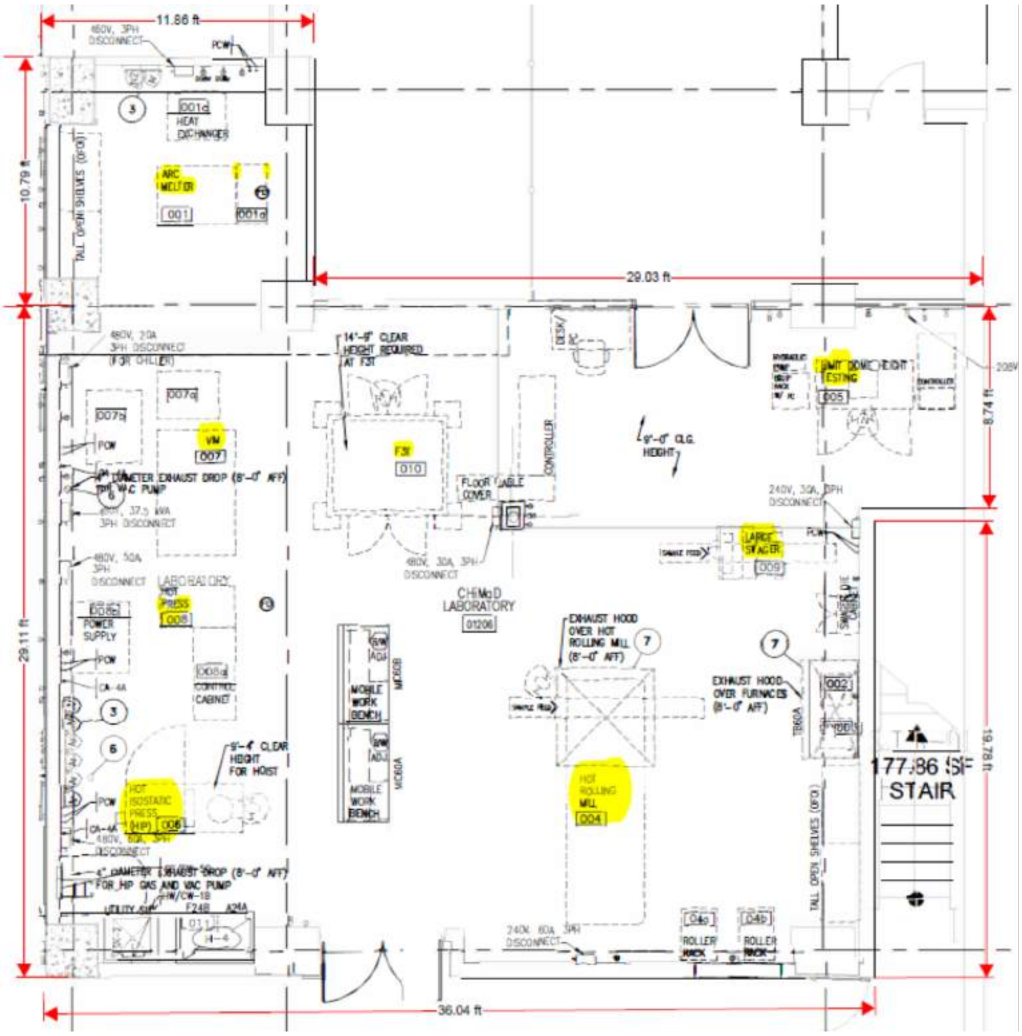


Figure 13.1: Plan of the CHiMaD Metals Processing Facility, designed with current and future equipment in mind.

Figure 13.2: *(left)* CHiMaD Materials Processing Facility as construction was completed, *(Right* The first equipment to be moved in was the Buehler AM/0.5 Arc Melter

Figure 13.3: *(Left)* Fenn 2/4 Hi Rolling Mill shown before refurbishing. *(Right)* A representation of how Fenn 2/4 Hi Rolling Mill is expected to look after refurbishing

Equipment Estimated to be Added During 2017

- 2 Vacuum Furnaces (Est. order: March 2017)
- 2 Box Furnaces (Est. order: March 2017)
- DAKE Horizontal Bandsaw (Est. order: April 2017)

Future Equipment

- Retech 30kg Vacuum Induction Melter (VIM)
- Hot Isostatic Press (HIP)
- Freeform Fabrication Technology (F3T)
- Sand/grit blaster
- Metal grinder

V

Outreach

14. CHiMaD Outreach Overview

The three pillars of the U.S. Government's Materials Genome Initiative (MGI) are:

1. Developing a open-access and open-source materials innovation infrastructure
2. Achieving national goals with advanced materials using this infrastructure
3. Equipping the next generation materials workforce in government, academia and industry.

CHiMaD outreach activities and workshops are designed and organized with these three major goals of the MGI in mind with an emphasis on training the current and next generation of government, industrial and academic researchers with the right tools to make MGI a sustainable success.

Towards this goal, in 2016, CHiMaD organized an MGI Seminar series, welcoming an international group of researchers to present about their MGI-related efforts as well as other international MGI initiatives they are a part of. This series of presentations were broadcast to all CHiMaD partner institutions. In accordance with the goal of equipping the next generation of researcher and in collaboration with ASM International Educational Committee, CHiMaD continued the dissemination of some of the most significant current materials design software to engineering universities in the U.S. where the universities are expected to build these tools into their undergraduate curriculum. In its first round in 2015, proposals by six universities were awarded, in 2016 this award was extended to three more universities. CHiMaD also took the lead in the organization of various high-impact workshops aiming at community building and bridging for collaborations and open-access exchange of knowledge on their topics of interest as well as initiated Materials Data and Database focused working groups and meeting series. Finally, CHiMaD in 2016 has been actively working on improving its outreach activities for under represented groups, working with high-school and undergraduate level students and through this, inspiring them to join the field. This chapter, therefore, provides an overview of the CHiMaD Outreach activities in 2016.

15. CHiMaD Supported MGI Seminars and Webinars

All CHiMaD seminar abstracts, presenter biographies and event fliers are available on the CHiMaD Event Archives at http://chimad.northwestern.edu/news-events/Event_Archives.html

02/08/16 - *CHiMaD HQ & Broadcast*
Introduction of Department of Materials and Chemistry at AIST
Norimitsu Murayama
Director General, Department of Materials and Chemistry, National Institute of Advanced Industrial Science and Technology (AIST), Japan

---

02/08/16 - *CHiMaD HQ & Broadcast*
Direct Computational Predictions Of Materials Functions Toward Materials Data Mining
Yoshihiro Asai
Research Center for Computational Design of Advanced Functional Materials, National Institute of Advanced Industrial Science and Technology (AIST), Japan

---

02/25/16 - *CHiMaD HQ & Broadcast*
Materials Design for Energy Applications
Marius Stan
Senior Computational Energy Scientist, Argonne National Laboratory

---

06/23/16 - *CHiMaD HQ & Broadcast*
Understanding "2-D Interfacial Phases" to Help Decipher the Materials Genome
Jian Luo
University of California, San Diego

07/22/16 - *CHiMaD HQ - Open Discussion*
Additive Manufacturing Efforts at NIST
Mark Stoudt
National Institute of Standards and Technology

09/02/16 - *California State Polytechnic University, Pomona*
Applications of Integrated Computational Materials Engineering and Materials Design

Ricardo K. Komai
CHiMaD Materials Design Efforts Coordinator
Olson Research Group, Northwestern University

09/15/16 - *TMS Data Curation Webinar Series*
Webinar 1: Overview of Data Curation Tools
Carelyn Campbell
National Institute of Standards and Technology

09/22/16 - *TMS Data Curation Webinar Series*
Webinar 2: Materials Data Facility
Ben Blaiszik
University of Chicago

09/29/16 - *CHiMaD HQ & Broadcast*
Active machine learning for high-throughput phase diagram determination from X-ray diffraction experiments
Gilad Kusne
National Institute of Standards and Technology

09/29/16 - *TMS Data Curation Webinar Series*
Webinar 3: Materials Commons
Brian Puchala and Glenn Tarcea
Department of Materials Science and Engineering, University of Michigan

10/03/16 - *CHiMaD HQ & Broadcast*
A Brief Introduction to the Materials Genome Institute of Shanghai University
On the Screen of Thermoelectric Materials: Chalcopyrites and Filled $CoSb_3$ as Examples
Wenqing Zhang
Materials Genome Institute, Shanghai University

10/06/16 - *CHiMaD HQ & Broadcast*
Developing a Robust 3-D Representation Framework for 3D Printed Materials
Edwin Schwalbach
Air Force Research Laboratory

10/06/16 - *CHiMaD HQ & Broadcast*
In Search of Unconventional Ultrathin Metastable Surface Oxides
Aloysius Soon
Department of Materials Science and Engineering, Yonsei University, Seoul, S. Korea

10/06/16 - *TMS Data Curation Webinar Series*
Webinar 4: Citrine Informatics
Kyle Michel
Chief Technical Officer, Citrine Informatics

10/13/16 - *Northwestern University*
The Materials Science and Engineering Prominent Alumni Series

---

Charlie Kuehmann
VP Materials Engineering, SpaceX and Tesla Motors

10/13/16 - *TMS Data Curation Webinar Series*
Webinar 5: Materials Data Curation System/Materials Resource Registry
Chandler Becker, Carelyn Campbell, and Zachary Trautt
National Institute of Standards and Technology

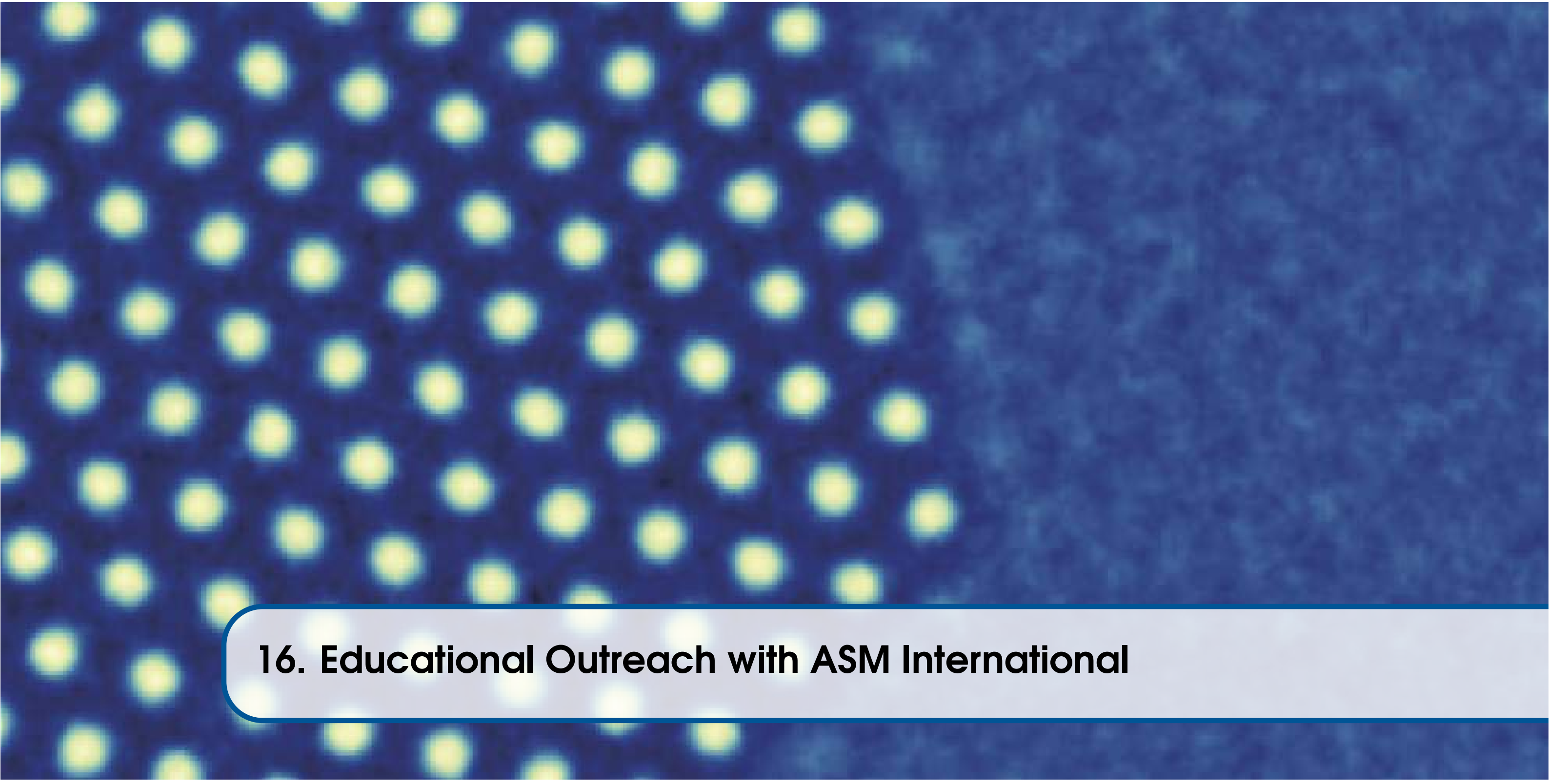
10/17/16 - *CHiMaD HQ & Broadcast*
Adventures in Flatland
Nicola Marzari
Theory and Simulation of Materials (THEOS)
National Centre for Computational Design and Discovery of Novel Materials (MARVEL)
Ecole polytechnique federale de Lausanne

10/28/16 - *CHiMaD HQ & Broadcast*
Multi-scale Microscopy: Can we connect the vision to reality?
Arno P. Merkle
Carl Zeiss Microscopy

11/10/16 - *CHiMaD HQ & Broadcast*
Hierarchical Materials Informatics for Accelerated Design, Development, and Deployment of Advanced Materials
Surya R. Kalidindi
Georgia Institute of Technology

12/09/16 - *CHiMaD HQ & Broadcast*
Functional Materials for Aerospace: Challenges and Opportunities
Richard A. Vaia
Functional Materials Division, Air Force Research Laboratory

12/16/16 - *CHiMaD Thesis Defense & Broadcast*
Machine Learning for Materials Discovery and Design
Logan Ward
Wolverton Research Group, Northwestern University



16. Educational Outreach with ASM International

16.1 ASM Materials Genome Toolkit

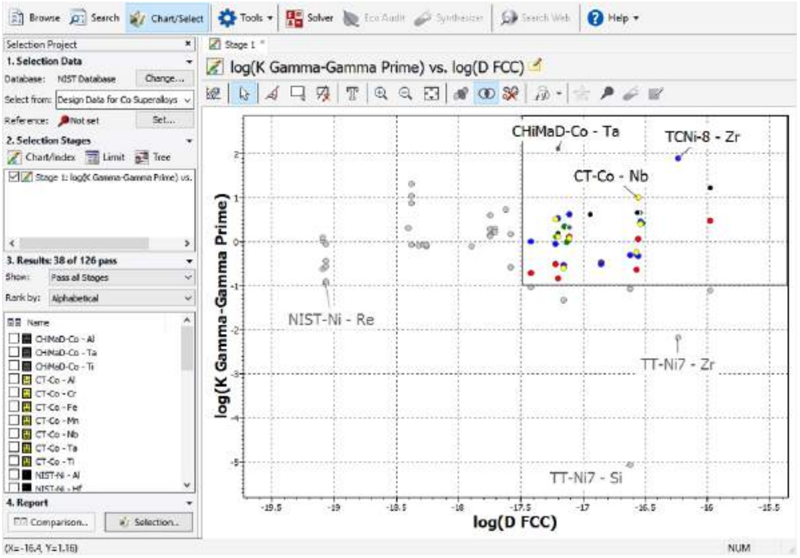
In 2015, ASM International and its affiliate members administered a competition among undergraduate universities in the U.S., awarding six schools with state-of-the-art materials design software and related materials property databases. The competition was announced in early 2015 and broadly publicized via direct email, on the ASM and CMD Network websites, through several ASM newsletters, and in a press release issued to various news outlets and materials-oriented professional societies. Schools competed on the basis of a proposal stating how they planned to integrate the Materials Genome Toolkit software into their undergraduate curriculum and in the context of the annual ASM Undergraduate Design Competition. A review committee convened by the ASM Action in Education Committee, the subcommittee on Computational Materials Engineering, evaluated the entries, ranking them according to several factors, including the degree to which the proposed plan balanced theory and application in the use of the software. In 2016, three more undergraduate-serving institutions were awarded the Materials Genome Toolkit .

To date, 11 institutions have received the three-year, multi-user license, giving hundreds of students and faculty across the U.S. access to the latest Thermo-Calc thermodynamics code, DICTRA multi-component diffusion code, TC-PRISMA precipitation simulator, and several thermodynamic and mobility databases. In 2016, the recipients of this award were Missouri University of Science & Technology, Case Western Reserve University and Oregon State University. In the first round of the competition in 2015, six engineering schools were selected to receive the Toolkit, including Alfred University, California State Polytechnic University in Pomona, Carnegie Mellon University, Michigan Technological Institute, the University of Maryland, and Virginia Polytechnic Institute and State University. An equivalent software package has also been awarded to the Colorado School of Mines, one of the top seven finishers in the toolkit competition, under the auspices of the Lightweight Innovations for Tomorrow (LIFT) consortium, and Fayetteville State University as a part of CHiMaD outreach for underrepresented groups in 2015. Refer to Figure 16.1 for a complete list of wining schools and the lead principal investigators of the proposals.

The CHiMaD-sponsored ASM Materials Genome Toolkit program is also made possible by Thermo-Calc Software, which generously offered an 85% discount on what will

ASM MGI Toolkit Awardees
Missouri University of Science & Technology (*2016 Awardee*) *Lead PI: Joe Newkirk, Department of Metallurgical and Materials Engineering* 3rd Place, 2016 ASM Undergraduate Design Competition
Case Western Reserve University (*2016 Awardee*) *Lead PI: David Matthiesen, Department of Materials Science and Engineering*
Oregon State University (*2016 Awardee*) *Lead PI: Julie D. Tucker, Department of Mechanical, Industrial and Manufacturing Engineering*
California State Polytechnic University in Pomona (*2015 Awardee*) *Lead PI: Vilupanur Ravi, Chemical and Materials Engineering* 1st Place, 2015 ASM Undergraduate Design Competition 1st Place, 2016 ASM Undergraduate Design Competition
Carnegie Mellon University (*2015 Awardee*) *Lead PI: Bryan Webler, Department of Materials Science and Engineering* 2nd Place, 2015 ASM Undergraduate Design Competition
Michigan Technological Institute (*Pilot Program*) *Lead PI: Paul Sanders, Department of Materials Science and Engineering* 3rd Place, 2015 ASM Undergraduate Design Competition
Alfred University (*2015 Awardee*) *Lead PI: S. K. Sundaram, Department of Materials Science and Engineering*
University of Maryland (*2015 Awardee*) *Lead PI: Yifei Mo, Department of Materials Science and Engineering*
Virginia Polytechnic Institute and State University (*2015 Awardee*) *Lead PI: Alan Druschitz, Department of Materials Science and Engineering*
Colorado School of Mines (*2015 Awardee*) **(*Awarded through LIFT*)** *Lead PI: Kip Findley, Department of Metallurgical and Materials Engineering*
Fayetteville State University (*2015 Awardee*) **(*Awarded through CHiMaD*)** *Lead PI: Alexander Umantsev, Department of Physics*

Figure 16.1: List of ASM MGI Toolkit Awardees in 2015 and 2016. The awarded schools took top three spots in the ASM Undergraduate Design Competition in 2015 and 2016; where Northwestern University was awarded 2nd place in 2016.



Database: NIST Database
Select from: Design Data for Co Superalloys
Reference: Not set
3. Results: 38 of 126 pass
Show: Pass all Stages
Rank by: Alphabetical

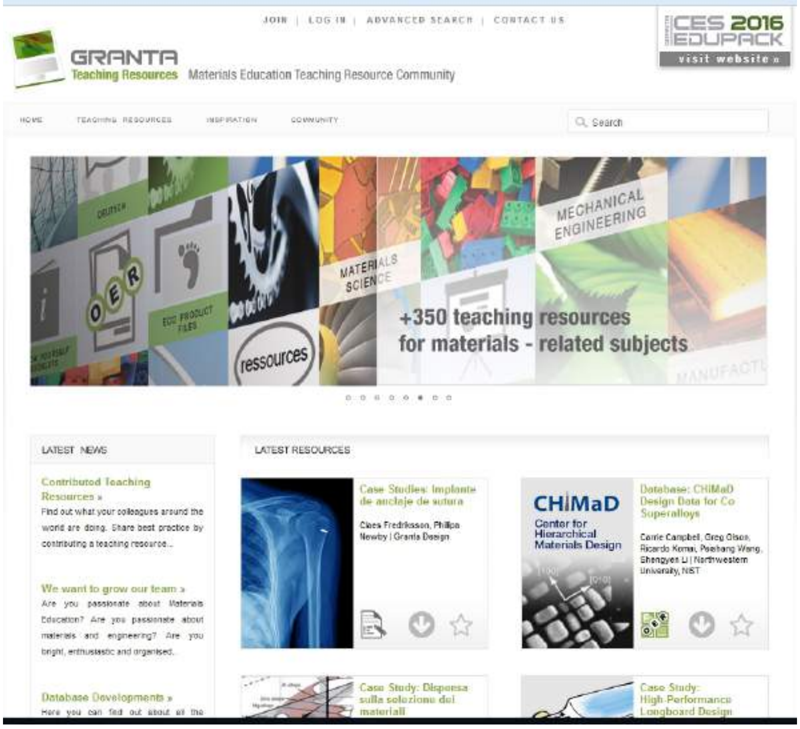
Figure 16.2: CHiMaD Data module at Teaching Resources Community website

ultimately be twelve sets of tools worth more than $1.6 million. The software distribution program addresses several CHiMaD objectives by helping the next generation of scientists and engineers become proficient with materials-by-design tools and techniques and by contributing to efforts that are advancing the collective knowledge on material systems and methodologies.

ASM will be conducting a third Materials Genome Toolkit competition in the coming year that will award up to three more undergraduate-serving engineering schools with state-of-the-art materials design software. The application deadline for the proposals is April 30, 2017. ASM is actively promoting the contest to faculty and students through email, newsletters, web posts, community forums, AM&P magazine, and a broadcast press release. ASM will also publicly recognize the first ten MGI toolkit winners during an ASM function at Materials Science and Technology 2016 in Salt Lake City, Utah, and will work to develop metrics to capture and convey how the toolkit program is benefitting each school.

16.2 Cobalt Phase Partitioning Database Development and Demonstration

CHiMaD PIs **Olson** (NU), **Campbell** (NIST) and postdoctoral researchers Komai (NU), Wang (NU-NIST) and Li (NIST), in collaboration with ASM (**Berardinis**, **Henry**) have engaged in an pilot effort to develop a shared resource for CHiMaD Use-Case Groups to manage and analyze protodata stemming from their work. As a first step, the collaborators built a database using the *Granta CES Selector* and populated it with Co phase partitioning data transmitted in the form of XML files. The ability to import data in XML format is a critical requirement for the new resource based on the anticipated workflow associated with protodata. Provisions for running accelerated searches are also required, and one of the reasons for using CES Selector in the initial development stage. ASM has demonstarted that the search tools on the CES platform could sort, filter, and plot the phase-based protodata, producing Ashby-type charts as seen in Figure 16.2.



Contributed Teaching Resources »
Find out what your colleagues around the world are doing. Share best practice by contributing a teaching resource...

We want to grow our team »
Are you passionate about Materials Education? Are you passionate about materials and engineering? Are you bright, enthusiastic and organised.

Database Developments »
Here you can fed out about all the

Case Studies: Implante de anclaje de sutura
Claes Fredriksson, Philipa Newby | Granta Design

Database: CHiMaD Design Data for Co Superalloys
Carrie Campbell, Greg Olson, Ricardo Komai, Peisheng Wang, Shengyen Li | Northwestern University, NIST

Case Study: Dispensa sulla selezione dei materiali

Case Study: High-Performance Longboard Design

Figure 16.3: CHiMaD Data module at Teaching Resources Community website

ASM and its partners also developed a lesson module based on the CHiMaD Cobalt database and placed it on the Materials Education Teaching Resource Community website, where it can be freely accessed by instructors and students around the world. The module, titled "CHiMaD Design Data for Co Superalloys," broadly promotes the instruction of integrated computational materials engineering (ICME) and the concepts of materials design. **Berardinis** (ASM) presented an early look at the landing page on the Teaching Resources Community website, Figure 16.3, during the 2016 CHiMaD Data and Analytics for Materials Research Summit. The site was selected because it offers the fastest and most economical route to disseminate the lesson module, exposing it to more than 10,000 academics around the world and over 300 institutions in North America.

16.3 Materials Genome Toolkit and Materials Design Training

In support of the integration of the MGI Toolkit software and materials design concepts into the undergraduate curriculum in recipient institutions, a 3-day MGI Toolkit and Materials Design training was organized by CHiMaD, ThermoCalc USA and hosted by Carnegie Mellon University on July 6-8, 2016, Figure 16.4. During the first two days of the workshop Mason (ThermoCalc USA) and Wu (ThermoCalc USA) lead the accelerated training for ThermoCalc, Prisma and Dictra software packages. To achieve this, attendees were given material to study prior to the workshop. Two representatives from each of the institutions awarded in 2015 attended the workshop, allowing for a small but hands-on workshop where different experience levels with the software could be accomodated, Figure 16.5. The training on the latter two software packages was found especially useful as most of the attendees used them for the first time. On the third day, a materials design training was lead by Komai (CHiMaD), Xiong (UPitt) and Gulsoy (CHiMaD), where attendees were given a broad overview of Systems Design Approach and CHiMaD. The workshop

Figure 16.4: CHiMaD/ThermoCalc MGI Toolkit and Materials Design Training attendees

was held in Pittsburgh, where ThermoCalc USA headquarters are located, and hosted by Carnegie Mellon University and its MGIToolkit award recipient Webler (CMU). A similar workshop is planned for summer of 2017 where awardees from 2016 competition as well as the previous year will be invited to train more educators and graduate students on the tools.

16.4 Collaborations

16.4.1 NIST Collaborations

Cobalt Phase Partitioning Database Development and Demonstration
Larry ***Berardinis*** *(ASM), Scott* ***Henry*** *(ASM), Gregory* ***Olson*** *(NU), Carelyn* ***Campbell*** *(NIST), Ricardo Komai (NU), Sheng Yen Li (NIST), Peisheng Wang (NU-NIST)*
The collaborators built a database using the Granta CES Selector and populated it with Co phase partitioning data developed by NIST researchers.

16.4.2 External Collaborations

Cobalt Phase Partitioning Database Development and Demonstration
Larry ***Berardinis*** *(ASM), Scott* ***Henry*** *(ASM), Stuart Dyer (Granta Design) and Tom Searles (MDMi)*
ASM, NIST and Northwestern PIs worked with representatives from Granta Design and MDMi to build and test the CES Selector database and develop the web page where a related lesson module resides.

Materials Genome Toolkit and Materials Design Training
Paul Mason (ThermoCalc USA), Ricardo Komai (CHiMaD), Wei Xiong (UPitt), Begum Gulsoy (CHiMaD), Bryan Webler (Carnegie Mellon University), Kevin Wu (ThermoCalc

Figure 16.5: CHiMaD/ThermoCalc MGI Toolkit and Materials Design Training setup

USA), Larry ***Berardinis*** *(ASM)*
In support of the integration of the MGI Toolkit software and materials design concepts into the undergraduate curriculum in recipient institutions, a MGI Toolkit and Materials Design training was organized. During the 3-day workshop Mason (ThermoCalc) lead the training for ThermoCalc, Prisma and Dictra softwares; Komai (CHiMaD), Xiong (UPitt) and Gulsoy (CHiMaD) lead the materials design training. The workshop was planned in close collaboration with Carnegie Mellon University and was hosted by CMU's recipient lead-PIs Webler (CMU). Two representatives from each of the institutions awarded in 2015 attended the workshop. A similar workshop is planned for summer of 2017.

Citrine Informatics
Larry ***Berardinis*** *(ASM), Scott* ***Henry*** *(ASM), Bryce Meredig (Citrine Informatics), Christina Hartman (Citrine Informatics)*
ASM PIs are collaborating with Bryce Meredig and Christina Hartman, exploring alternate methods for browsing, viewing, and mining materials data. As a first step, ASM provided Handbook data to Citrine, which it uploaded to its software platform for review. Pending a successful outcome, the next round of testing will focus on microstructure images and data, potentially progressing to 3D datasets that may be of interest to particular CHiMaD Use-Case Groups.

16.5 Technology Transfer

Database
CHiMaD Design Data for Co Superalloys
T. J. Brown, S. Dyer
Date: 10/28/16
Distribution: Public

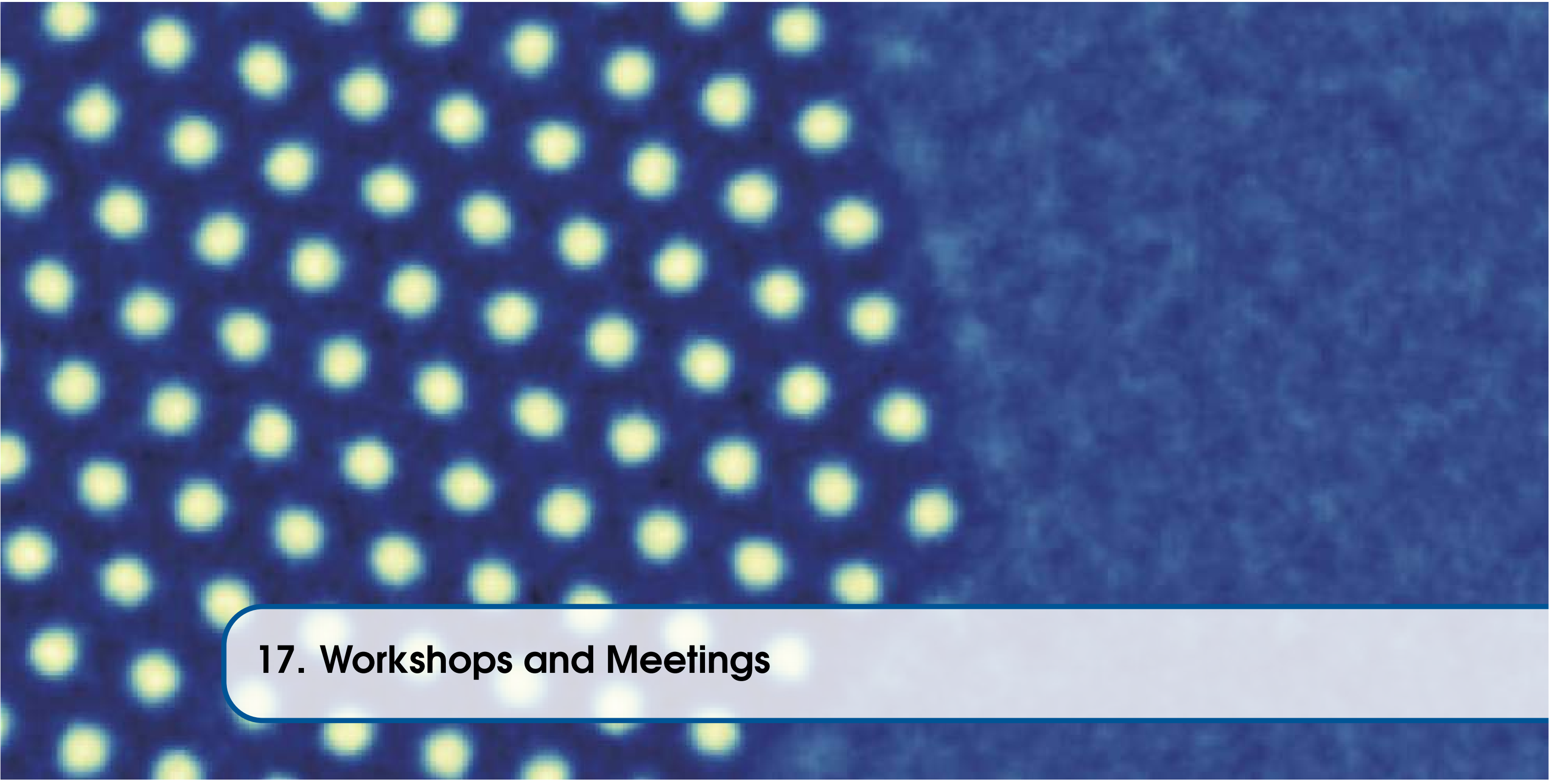
Link: http://teachingresources.grantadesign.com/Mechanical_Engineering/GDBCHIEN16
ASM International, with support from MDMi and Granta Design, built a database in CES Selector using Cobalt phase partitioning data provided by NIST and Northwestern University. The database served to demonstrate that the search-selection tools in CES Selector could adequately sort and display low-level data, representative of modeling data derived using CALPHAD tools and methods. It is also the central element in a lesson module intended for teaching materials design.

16.6 Publications and Presentations

6 Number of e-newsletters and press releases on CHiMaD collaborations in 2016 by ASM group. Please see chapter 24.14 for details.

16.7 ASM Team

ASM **Technical Staff**			
Name	**Position**	**Affiliation**	**Project** (PI)
Larry Berardinis	Senior Manager, CMD Network	ASM	ASM Materials Genome Toolkit, Data Search-Selection Tools
Scott Henry	Senior Content Engineer	ASM	ASM Materials Genome Toolkit, Data Search-Selection Tools



17. Workshops and Meetings

17.1 CHiMaD Thermoelectric Design Workshop

February 29, 2016 | *Organizer: Gregory* ***Olson*** *(NU), QuesTek*

Scope

Thermoelectric materials could play a key role in meeting increasing global energy needs, but are currently limited due to their low efficiency. Current research is dedicated to investigating methods for improving their overall efficiency.

Northwestern University's SRG design consortium founded in 1985 now operates under CHiMaD auspices with the materials design research projects including the DARPA-SIMPLEX project integrating data analytics with microstructural design of thermoelectric materials. Work by **Voorhees** (NU) and Peters (NU-supported by NDSEG Fellowship), has been focused on building thermodynamic models and databases through the CALPHAD method to be used in optimizing Pb-based thermoelectric systems in collaboration with QuesTek and supported partially by the DARPA-SIMPLEX project in 2016.The *CHiMaD Thermoelectric Design Workshop* was organized on February 29, 2016 to further present current capabilities, interests as well as explore possible future directions and collaborations within CHiMaD institutions regarding thermoelectric materials. Following presentations were given during the workshop:

- CHiMaD Introduction and Efforts, *Gregory* ***Olson*** *(NU)*
- Thermoelectrics Overview, *Jeffrey Snyder (NU)*
- Synthesis of Thermoelectrics, *Mercouri Kanatzidis (NU)*
- Transverse Thermoelectrics, *Matthew Grayson (NU)*
- DARPA SIMPLEX, *James* ***Saal*** *(QuesTek)*

17.2 CHiMaD Materials Design Workshops

March 3-4, 2016 | *Organizers: Ricardo Komai (NU), Begum Gulsoy (NU)*
June 13-14, 2016 | *Organizers: Gregory* ***Olson*** *(NU), Carelyn* ***Campbell*** *(NIST), Ricardo Komai (NU)*

Scope

The *CHiMaD Materials Design Workshop* series aims to enhance the understanding of *Materials by Design* concepts by CHiMaD graduate students and postdoctoral researchers and to have them better understand how and where their research fits within the design goals of the use-cases they are working with.

The goal of the first two-day community-building workshop in 2015 was to form a Systems Design Chart for CHiMaD use-case on both hard and soft materials. This effort was very beneficial for the students and postdocs in furthering their understanding of *Materials by Design* concepts and for identifying the unique materials design goals for each use-case group and its projects. A follow-up workshop was organized on March 3-4, 2016; it was designed to refine the systems design charts built on the first workshop and to identify the sub-systems within these design charts that correspond to each student and postdocs research. The workshop had 21 attendees who worked to refine four of the system design charts.

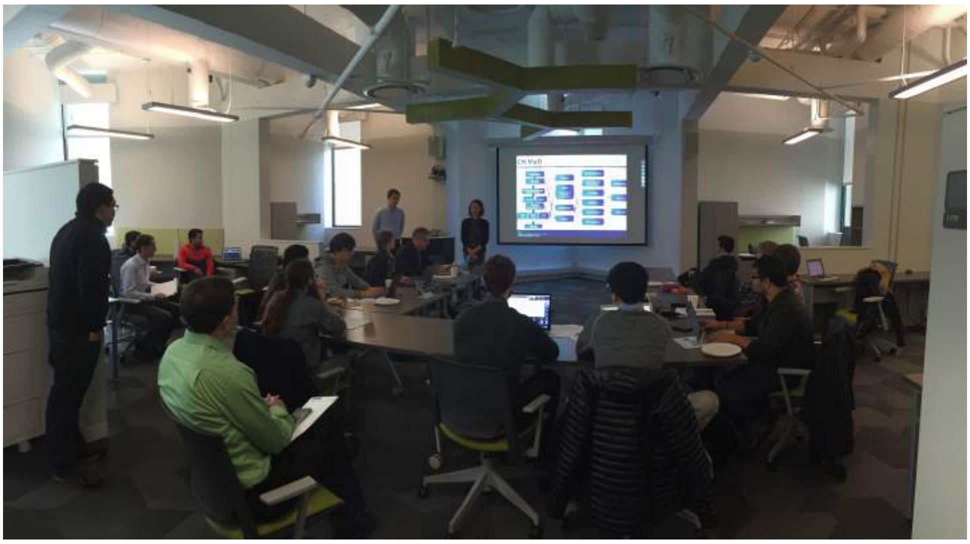


Figure 17.1: Hadallia Bergeron (NU) from **Hersam** (NU) research group presenting the refined Low-Dimensional Nanoelectronic Materials use-case group systems design chart

The 3^{rd} *CHiMaD Materials Design Workshop* was organized at NIST, with the NIST lead organizer as **Campbell** (NIST). This workshop, in contrast to the first two, was organized for CHiMaD's NIST colleagues and the keynote was given by Gregory **Olson** (NU). During this workshop, 25 of CHiMaD's NIST colleagues had a chance to explore the *Materials by Design* concepts in a similar hands-on fashion and worked on building existing systems design charts as well as in some cases enhancing those previously built by CHiMaD students and postdoctoral researchers. Such cases were a good example of using different levels of expertise in refining the systems design charts.

17.3 32nd Steel Research Group (SRG) Meeting

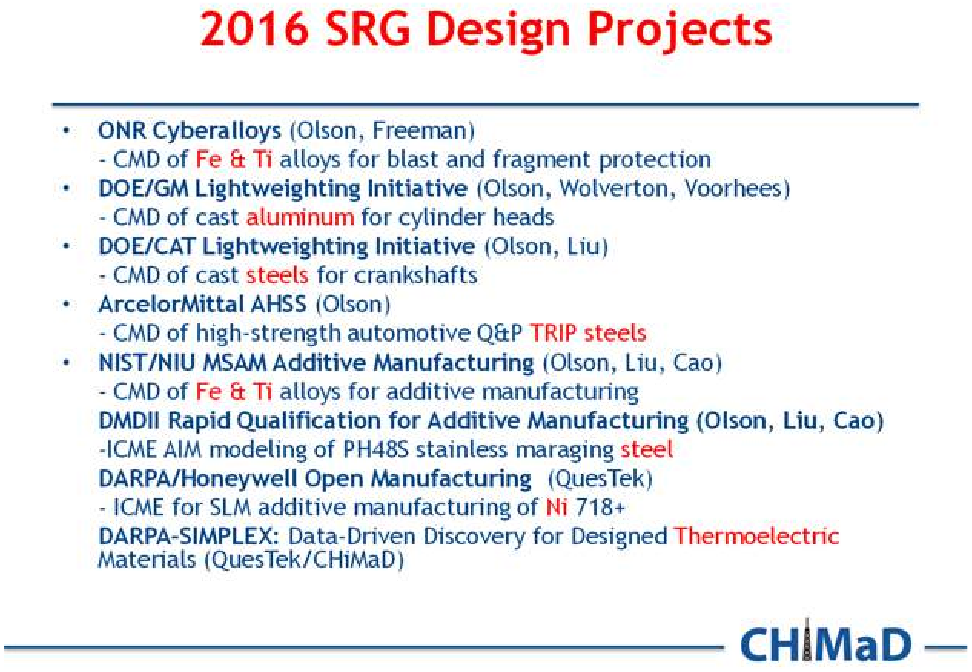
March 21-22, 2016 | *Organizer: Gregory **Olson** (NU)*

organized in conjunction with
NU-NIMS for Materials Innovation: Joint MGI Workshop
March 24, 2016 | *Organizer: Gregory **Olson** (NU)*

Scope
Northwestern's Steel Research Group (SRG) materials design consortium joined the CHiMaD umbrella organization during Year One, offering the leveraging opportunity of the CALPHAD-based metals design projects with topics and sponsors listed in Figure 17.2.

Of particular note in 2016 was the experimental validation of phase relations in a designed TRIP Titanium alloy optimized for transformation toughening. The collaboration with GM under the DOE Lightweighting Initiative has further quantified the thermodynamics and kinetics of Q phase precipitation strengthening and applied it in design of cast Al alloys with higher temperature performance. Caterpillar collaboration under the same DOE initiative has adapted multiphase precipitation concepts from our previous martensitic blast protection steel designs to demonstrate novel cast steel prototypes for lower cost crankshaft applications. AHSS design research supported by ArcelorMittal is quantifying the nonequilibrium thermodynamics of carbon partitioning in Quench & Partition martensite-austenite TRIP steels for high formability automotive sheet applications. In support of the new process technology of additive manufacturing, the NIST-MSAM project completed in 2016 has quantified recrystallization behavior of Ti and steel alloys, while a new project under the Chicago-based DMDII Manufacturing Institute is applying the results in rapid qualification strategies demonstrated with QuesTek's Ferrium PH48S stainless maraging steel. QuesTek's collaboration with Honeywell under the DARPA Open Manufacturing initiative continues to support AIM qualification of printed Ni superalloy components for aerospace applications. Building on our CHiMaD Year One demonstration of a hybrid approach to integrating CALPHAD with datamining techniques, QuesTek secured a major DARPA consortium project with CHiMaD to apply this approach to integrated compound discovery and predictive microstructural design in thermoelectric materials. These projects will help demonstrate the generality of the methods, tools, and database infrastructure of CHiMaD. The SRG Annual Meeting held each March at Northwestern continues to serve as a review of CHiMaD metals activities offering interaction with a broader community. In support of NIST collaboration, NIST speakers at the 2016 SRG meeting included J. **Warren**, C. **Campbell**, E. **Lass** and M. **Stoudt**.

Building on the NIST-sponsored US/Japan Materials Genome Workshop held in Tsukuba in June 2015, the 2016 SRG meeting at Northwestern was followed by the 4th NU-NIMS Materials Genome Workshop. Plans for enhanced collaboration between NU and NIMS continue, with the Materials Genome Workshop now an annual event.



2016 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

DMDII Rapid Qualification for Additive Manufacturing (Olson, Liu, Cao)
-ICME AIM modeling of PH48S stainless maraging steel
DARPA/Honeywell Open Manufacturing (QuesTek)
- ICME for SLM additive manufacturing of Ni 718+
DARPA-SIMPLEX: Data-Driven Discovery for Designed Thermoelectric Materials (QuesTek/CHiMaD)

CHiMaD

Figure 17.2: Steel Research Group (SRG) 2016 projects related to precipitation-strengthened alloys and design.

17.4 CHiMaD Annual Review Meeting

March 24, 2016 | *Organizers: Peter **Voorhees** (NU), Gregory **Olson** (NU), Juan **de Pablo** (UC), Begum Gulsoy (NU)*

Scope

The *The CHiMaD Annual Review Meeting is the technical overview of the Center for Hierarchical Materials Design. It annually brings together CHiMaD principal investigators, postdoctoral researchers and students from Northwestern University, University of Chicago, Argonne National Laboratory and Fayetteville State University as well as partners from QuesTek Innovations and ASM International along with collaborators from National Institute of Standards and Technology. This meeting also acts as a platform for the CHiMaD Technical Advisory Board to review and provide feedback on the CHiMaD activities and for industrial partners to explore the capabilities of and possible partnerships with CHiMaD.*

In 2016, the *CHiMaD Annual Review Meeting* was attended by 139 people including researchers affiliated with CHiMaD institutions and QuesTek Innovations, 25 attendees friom NIST, and 14 from NIMS, Japan, Figure 17.3. Industrial companies represented included *Dow, IBM Research, imec, Intel Corporation, Marc Inc, Pratt & Whitney, Solvay, SpaceX, Tesla Motors*, who are members of CHiMaD Technical Advisory Board, as well as *Goodyear*, a collaborator of Polymer Matrix Materials use-case group. Techical presentations of the use-case groups were lead by the corresponding use-case leaders. During the CHiMaD Annual Review Meeting Poster Session, 32 posters were presented by CHiMaD students and postdoctoral researchers, where the attendees had a chance to

Figure 17.3: Ankit **Agrawal** (NU) presenting on CHiMaD Data Mining effort during the *CHiMaD Annual Review Meeting*.

directly inquire about the specific projects the students are researching on.

17.5 CHiMaD Phase Field Methods Workshop III & Hackathon

May 3-5, 2016 | *Organizers: Olle* ***Heinonen*** *(ANL), Peter* ***Voorhees*** *(NU), James* ***Warren*** *(NIST) and Jonathan* ***Guyer*** *(NIST)*

Scope

The goal of the CHiMaD Phase Field Methods Workshop series is to develop the first-set of benchmark problems for the global phase field community and to engage this elite team of invited experts for in providing input during this development.

Heinonen (ANL), **Voorhees** (NU), **Warren** (NIST) and **Guyer** (NIST), along with postdoctoral researchers Jokisaari (NU-ANL) and Keller (NIST), have brought together an elite team of Phase Field experts and framework developers during CHiMaD Phase Field Methods Workshops I-III, Figure 17.4. The first workshop was organized on January 9, 2015; the second one, along with the first *CHiMaD Phase Field Methods Hack-a-thon*, was organized on October 15-16, 2015. The third workshop and hack-a-thon in the series took place on May 3-5, 2016. The goal of these workshops was to develop the first-set of benchmark problems for the global phase field community and to engage this elite team of invited experts for in providing input during this development. On that end, Hack-a-thons have been organized in Workshops II-III where students, postdoctoral researchers and experts have gotten a chance to tackle the drafted benchmark problems. The first set of benchmark problems for the Phase Field community has been published in *Computational Materials Science* [25.30], and has been selected as the Editor's Choice. The published benchmark problems have been constructed based on the discussion and feedback during the CHiMaD Phase Field Workshops. The benchmark problems, together with one set of solutions, have been made available online for the community at the CHiMaD Phase Field Website developed by Wheeler (NIST) and can be accessed at *(https://pages.nist.gov/chimad-phase-field/#benchmarks)*. It is expected that these benchmark problems will be a significant resource for developers of phase field codes - the problems are already being used in

Figure 17.4: Attendees of the *CHiMaD Phase Field Methods Workshop III & Hackathon*

college courses taught by CHiMaD Phase Field Methods workshop contributors such as by Michael Tonks (Penn State). A second set of benchmark problems are in preparation and will be tested in 2017 during CHiMaD Phase Field Methods workshops IV-V. For extended information on CHiMaD's effort in Phase Field Methods, please refer to section 11.

17.6 NIST Additive Manufacturing Workshop

May 23-24, 2016 | *Local Organizers: Jian* ***Cao*** *(NU), Wing Kam* ***Liu****, Gregory* ***Olson****, Kornel Ehmann (NU)*

Scope

The scope of the "NIST Additive Manufacturing Workshop on Measurement Science for Directed Energy Deposition" is to identify needs, establish priorities, and develop action plans to advance capabilities for additive manufacturing by directed energy deposition.

NIST Additive Manufacturing Workshop: Measurement Science for Directed Energy Deposition took place on May 23-24, 2016 at Northwestern University, hosted by the Northwestern Initiative for Manufacturing Science & Innovation (NIMSI) with 74 attendees. This event brought together experts from diverse stakeholder groups to identify current and future needs, establish priorities, and develop action plans to advance the capabilities for metal-based additive manufacturing by Directed Energy Deposition. Directed Energy Deposition (DED) is a type of additive manufacturing process in which focused thermal energy is used to fuse materials (either in metal powder or solid stock form) by melting them as they are being deposited. Several commercial and research systems exist to produce metal parts using this approach. This workshop built on prior additive manufacturing roadmaps and other efforts that have identified technology challenges and R&D needs, and will focus on high-priority measurement science needs. Workshop objectives were to identify:

- Measurement science barriers, challenges, and gaps that prevent the broad use of directed energy deposition processes
- Priorities and timing for corresponding additive manufacturing standards development
- R&D needs to address the priority measurement and standards challenges

The workshop included a panel discussion and facilitated break-out sessions to define the requirements and priorities. The break-out sessions concentrated on (1) Process Measurement, Modeling, and Control and (2) Feedstock Materials and Mechanical Properties.

17.7 Impact Mitigating Materials for Body Protection Workshop

August 8, 2016 | *Organizers: Aaron **Forster** (NIST), Juan **de Pablo** (UC), Chelsea **Davis** (NIST), Sidney **Nagel** (UC), Heinrich **Jaeger** (UC)*

Scope

The scope of the "Impact Mitigating Materials for Body Protection Workshop" is to identify current state-of-the-art in test-method development and injury thresholds; to identify methodologies to correlate material structure and dynamic properties to performance improvements from blunt impacts, ballistic, and blast protection; and to identify ways Materials by Design concepts could accelerate innovation and reduce injury rates.

On August 8, 2016 CHIMaD and NIST hosted an Impact Mitigating Materials for Body Protection Workshop at the University of Chicago. This intimate workshop, 30 attendees, brought together leaders from academia and government in the areas of biomechanics, high-rate impact testing, and standard test methods for protective equipment. The discussion on injury criteria and ideal material response characteristics aim at developing measurement strategies for desirable material properties and system performance in order to create novel impact mitigating materials by design. The workshop featured seven invited speakers from ARL, Virginia Tech, Johns Hopkins, UCLA, Carleton, Under Armour, and the Consumer Safety Commission as well as speakers from NIST and UC.

The workshop hosted seven invited speakers from ARL, Virginia Tech, Johns Hopkins, UCLA, Carleton, Under Armour, and the Consumer Safety Commission as well as speakers from NIST and UC. The first session focused on the latest test methods for evaluating helmet performance in military and sports applications, with a presentation on innovative methods to structure materials to improve ballistic performance. The second session focused on the methodology used to understand an injury mechanism, experimentally recreate/validate the mechanism, and transition to a standard test method.

The materials-by-design approach to impact mitigation challenges is composed of novel dynamic-impact metrologies and novel, engineered energy-dissipation mechanisms for multi-material systems that are supported by new materials models. This perspective was a template for the afternoon group discussion topics on:

- Injury Criterion and Ideal Material Response
- Measurement Strategies for Material Properties and System Performance
- Materials by Design

For a broader overview of CHiMaD's Impact Mitigation Efforts and this workshop, please see the Impact Mitigation Seed Group Report on Chapter 9.

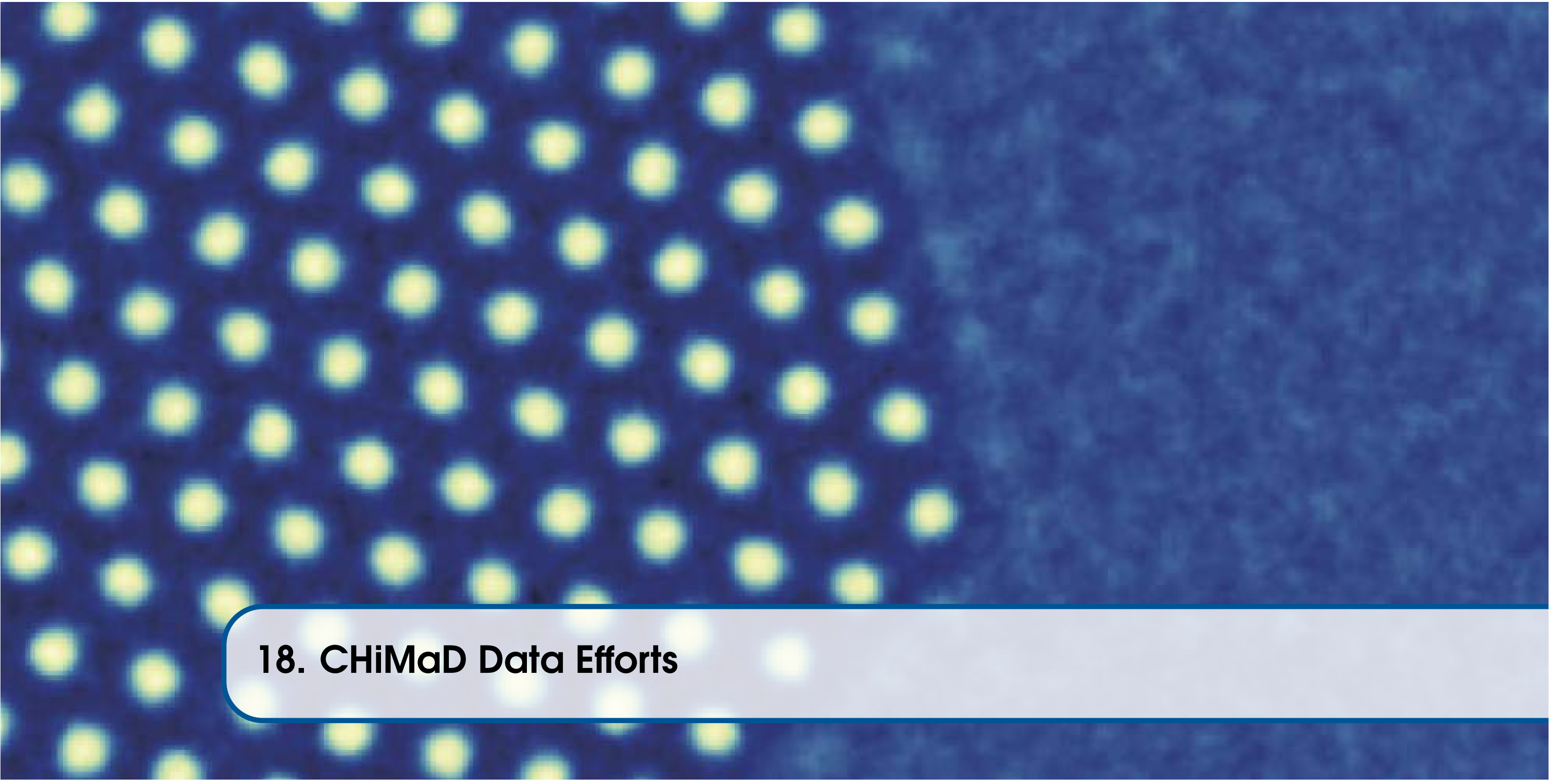
17.8 Other Outreach Activities Organized by CHiMaD PIs in 2016

A Workshop on Predictive Theoretical and Computational Approaches for Additive Manufacturing
October 7-9, 2015 | National Academies, Washington DC | *Organizer: Wing Kam* ***Liu*** *(NU)*
NIST Presenters: Richard Ricker (NIST), Li **Ma** (NIST), Lyle **Levine** (NIST)
CHiMaD Presenters: Jian **Cao** (NU)

October 16-19, 2016 | Dalian, China | *Organizers: Wing Kam* ***Liu*** *(NU), Lyle* ***Levine*** *(NIST), Richard Ricker (NIST)*
NIST Presenters: Lyle **Levine** (NIST)

The 2015 workshop, conceived and organized by Professor Liu, was funded by the National Science Foundation, the National Institute of Standards and Technology, and Sandia National Laboratories, at the National Academies' Keck Center in Washington, DC. The details of the workshop along with the a copy of the presentations are available online [http://sites.nationalacademies.org/PGA/biso/IUTAM/PGA_168737]. As a result of this workshop, **Liu** (NU) and **Levine** (NIST) have proposed a series of benchmark tests and an accompanying conference series with the aim to develop AM standards. In 2016 the first follow-up workshop was organized by Wing Kam **Liu** (NU), Lyle **Levine** (NIST), Richard Ricker (NIST).

Principles of Directed Self-assembly (DSA)
February 2016 | SPIE Advanced Lithography Conference, San Jose, CA | *Organizer: Paul* ***Nealey*** *(UC)*
An SPIE Short Course on Principles of Directed Self-assembly was taught by **Nealey** (UC) during the SPIE Advanced Lithography Conference.



18. CHiMaD Data Efforts

Laura Bartolo (NU), Ankit Agrawal (NU), Cate Brinson (NU), Juan de Pablo (UC), Ian Foster (UC), Peter Vorhees (NU), Benjamin Blaiszik (ANL), Richard Zhao (NU), Begum Gulsoy (NU)

James Warren (NIST), Carelyn Campbell (NIST), Zachary Trautt (NIST), Chandler Becker (NIST), Frederick Phelan (NIST), Debbie Audus (NIST), Ursula Kattner (NIST), Kenneth Kroenlein (NIST), Shengyen Li (NIST), Raymond Plante (NIST), Alden Dima (NIST), Sharief Youssef (NIST)

Significance

Digital data and a materials innovation infrastructure are foundational components of the Materials Genome Initiative for accelerating discovery of new materials and reducing costs of advanced manufacturing. NIST plays a central role in the Federal government on the establishment of the materials innovation infrastructure to enable effective data exchange; best practices for data quality; and analytics for data-driven materials science. As the NIST Center of Excellence for Hierarchical Materials Design, CHiMaD concentrates its data efforts on collaboration, contribution and implementation to data exchange, data management practices, and data-driven materials science analytics to meet the goals of the Center and NIST.

18.1 Goals

Effective data tools, best practices, and standards are required for CHiMaD and others in the materials community to capitalize on the benefits of a robust materials innovation infrastructure to reach the goals of MGI. To meet this need, CHiMaD works in concert with NIST and others in the materials community on development and adoption of tools, best practices, and standards. The first year of CHiMaD's data efforts to integrate data management into scientific practices has focused on two primary areas: 1) workshops, training sessions, and working groups to increase awareness and knowledge of the current materials data landscape; and 2) collaborations across the Center, with NIST, and with others in the materials community to increase the potential for impact and adoption of promising advances.

To support data tool development, best practices, and standards, CHiMaD held multiple workshops, training sessions, working groups meetings, as well as established the CHiMaD/MDF instance of the NIST Materials Resource Registry in 2016. Presentations from these workshops are available to view on the CHiMaD Website.

18.2 CHiMaD Data Workshops

Data, Databases, & Discovery Workshop

On January 25, 2016, CHiMaD and NIST ran the first of three data workshops. "Data, Databases, & Discovery Workshop" was an internal event to support CHiMaD/NIST joint Use Cases and related data initiatives. Fifty-eight CHiMaD and NIST collaborators took part in the general sessions and 5 separate working group sessions during the one-day workshop. Working groups were established in the following topics:

- Working Group 1: MDCS, DSpace, MRR and MDF
- Working Group 2: Experimental Data
- Working Group 3: Schemas for Polymer Nanocomposite Data
- Working Group 4: Natural Language Processing
- Working Group 5: DFT
- Working Group 6: Building CALPHAD proto-databases

Building an Interoperable Materials Data Infrastructure

To broaden its impact and partnerships, CHiMaD held the second data workshop on May 2, 2016, "Building an Interoperable Materials Data Infrastructure", with major US data tool developers and data centers participating. Forty-five participants from twenty-four university, government, and industry research labs took part in the one-day event with 18 developers giving brief presentations, Figure 18.1. The following national data efforts were presented:

- Materials Data Facility, *Ian **Foster**, University of Chicago*
- nanoHUB, *Gerhard Klimick, Purdue University*
- HUBzero, *Michael Zentner, Purdue University*
- Materials Project, *Qimin Yan, LBNL*
- Materials Data Curator System, *Sharief **Youssef**, NIST*
- Materials Commons, *Brian Puchala, University of Michigan*
- National Data Service, *Kenton McHenry, NCSA*
- ICE system, *Matt Jacobsen, AFRL*
- Citrine, *Bryce Meredig, Citrine Informatics*
- MAterials Simulation Toolkit (MAST), *Tam Mayeshiba, University of Wisconsin*
- Open Quantum Materials Database (OQMD), *Vinay Hedge, Logan Ward, Northwestern University*
- Harvard Clean Energy Project, *Alan Aspuru-Guzik, Harvard University*
- AFLOWLIB, *Cormac Toher, Duke University*
- Timely and Trusted Curation/Coordination (T2C2), *Steve Konstanty, University of Illinois*
- Two-Dimensional Crystal Consortium (2DCC-MIP), *Vin Crespi, Pennsylvania State*
- Analysis, Discovery of Interface Materials (PARADIM-MIP), *Lynn Rathbun, Cornell University*

Figure 18.1: Attendees of CHiMaD Building an Interoperable Materials Data Infrastructure Workshop on May 2, 2016

- Midwest Integrated Center Computational Materials (MICCoM), *Marco Giovoni, ANL*
- Materials Resource Registry, *Ray **Plante**, NIST*

To facilitate targeted result-driven discussions, working groups were established in the following topics:

- Working Group 1: Materials Research and Design
- Working Group 2: Tools and services "Necessary for the completion of work...Allows access and manipulation... Is intended to be easily usable"
- Working Group 3: Infrastructure "Underlying foundation or basic framework", Data Infrastructure "A digital infrastructure promoting data sharing and consumption"
- Working Group 4: Interoperability - The ability of systems to exchange and use information from other systems

2016 Data Summit on Materials Data and Analytics for Materials Research

The third workshop culminated the 2016 CHiMaD data series on October 31-November 2, 2016 with the "2016 Data Summit on Materials Data and Analytics for Materials Research", Figure 18.2. "Challenges in Data Design for Emerging Reconfigurable Soft Materials" session of the Summit was co-sponsored by NSF. Ninety-five participants took part from thirty-five university, government, and industry research labs and six countries. A follow up survey with 40% response rate of Summit participants indicated good support for the meeting. Bringing together an international materials data community, the meeting was organized into keynote talks and panels on the following topics:

- **Innovations in Materials Design:** Gregory **Olson** (NU), Juan **De Pablo** (UC) *Moderator: Ian **Foster** (UC/ANL)*
- **Data Curation:** John Allison (University of Michigan), Claudia Draxl (Humboldt University of Berlin) *Moderator: Chandler **Becker**, NIST*

Figure 18.2: CHiMaD Director Juan **de Pablo** (UC) speaking at the 2016 Data Summit on Materials Data and Analytics for Materials Research

- **Materials Analytics:** Elizabeth Holm (Carnegie Mellon University), Jed Pitera (IBM) *Moderator: Begum Gulsoy, CHiMaD*
- **Education, Workforce Development, Diversity, & Industry:** Katsuyo Thornton (University of Michigan), Alejandro Strachan (Purdue University) *Moderator: Marius* ***Stan*** *(ANL)*
- **Sustainability, Public/Private Partnerships, & Industry:** David Furrer (Pratt & Whitney), Bryce Meredig (Citrine) *Moderator: Ben Blaiszik (ANL)*
- **Challenges in Data Design for Emerging Reconfigurable Soft Materials:** Marcus Muller (University of Gottingen), Christopher Spadaccini (Lawrence Livermore National Laboratory), Alexander Hexemer (Lawrence Berkeley National Laboratory) *Moderator: Juan* ***De Pablo*** *(UC)*
- Education, Workforce Development, Diversity & Industry Panel: Begum Gulsoy (CHiMaD), Elif Ertekin (U of Illinois), Larry Berardinis (ASM) *Moderator: Begum Gulsoy, CHiMaD*
- Sustainability, Public/Private Partnerships, & Industry Panel: Ian **Foster** (UC/ANL), Bryce Meredig (Citrine), Arno Merkle (Zeiss), Charles Ward (AFRL) *Moderator: Jason* ***Sebastian****, QuesTek*
- Introduction to Materials Analytics Introduction & Current Efforts Session: Ankit **Agrawal** (NU), Turab Lookman (Los Alamos National Laboraory), Amanda Petford-Long (ANL)
- Working Group 1: Overview of Materials Data Curation Tools (Leads: Carelyn **Campbell** (NIST), Laura Bartolo (CHiMaD), Ben Blaiszik (ANL))
- Working Group 2: International Federation of Materials Resource Registries (Lead: Chander **Becker** (NIST)
- Working Group 3: Refining Preliminary Materials Data Schemas (Leads: Carelyn **Campbell** (NIST), Zachary **Trautt** (NIST)

A hands-on demo sessions was also organized as a part of the Summit, where the following data efforts were presented: ASM, Citrine, MagPie, Materials Data Facility,Materials Resource Registry, Materials Data Curator System, National Data Services, NanoHub, NanoMine, NIMS MatNavi,NoMaD, OQDB.

Figure 18.3: Attendees of Data Schema & MDCS Training on May 3, 2016

18.3 Support for & Contribution to NIST Data Schema efforts

In addition to workshops, CHiMaD researchers participated in data schema development events that the Center co-hosted with NIST; implemented the CHiMaD/MDF instance of the NIST Materials Resource Registry; and submitted an NSF proposal for the Midwest Big Data Spoke to extend the reach of NIST data schemas.

Data Schema & MDCS Training

CHiMaD co-hosted and participated in a one-day training session on the Materials Data Curation System (MDCS) and data schema development for specific subgroups as well as the Materials Data Facility (MDF) for CHiMaD researchers and their students on May 3, 2016 at CHiMaD HQ, Figure 18.3.

Summer Data Schema Development Working Groups

During Summer 2016, CHiMaD researchers and students worked closely with NIST's lead on data schema developments for particular research areas: DFT and computational; Mechanical testing and thermomechanical processing; Phase equilibria, diffusion, thermal analysis; and Polymers. Each area held three one-hour teleconference calls lead by Zachary **Trautt** (NIST) and Carelyn **Campbell** (NIST) that focused primarily on reviewing the Materials Data Curation Systems, the concept of modular schemas, and the current state of applicable schemas. Participants in the teleconference calls contributed Use Cases and datasets.

TMS Webinar Series on Data Curation

CHiMaD was one of the main supporters of the 5-week long TMS Webinar series on Data Curation which started in Septermber 2016. The efforts to organize this webinar series was lead by the TMS ICME Committee and in particular by Carelyn **Campbell** (NIST). This series highlighted data efforts and resources developed by NIST and CHiMaD among others. The following data tools were presented:

1. *Webinar 1:* Overview of Data Curation Tools, Carelyn **Campbell** (NIST)
2. *Webinar 2:* Materials Data Facility, Ben Blaiszik (UC)
3. *Webinar 3:* Materials Commons, Brian Puchala and Glenn Tarcea (University of Michigan)
4. *Webinar 4:* Citrine Informatics, Kyle Michel (Citrine Informatics)
5. *Webinar 5:* Materials Data Curation System and Materials Resource Registry, Chandler **Becker** (NIST), Carelyn **Campbell** (NIST), and Zachary **Trautt** (NIST)

CHiMaD/MDF instance of Materials Resource Registry

CHiMaD launched its instance of the NIST Materials Resource Registry Curation System (MRR) on October 31, 2016. The CHiMaD/MDF MRR provides high level metadata about CHiMaD resources (data collections, organizations, large data sets, services, informational sites, and software). The MRR and its resource records will enable the outside materials community to discover, promote, and access the CHiMaD researchers and their output. The CHiMaD/MDF MRR is taking part in discussions to establish an international federation of materials resource registries. Also see section 10.6, "Cloud Deployment of a MDF Materials Resource Registry (MRR)".

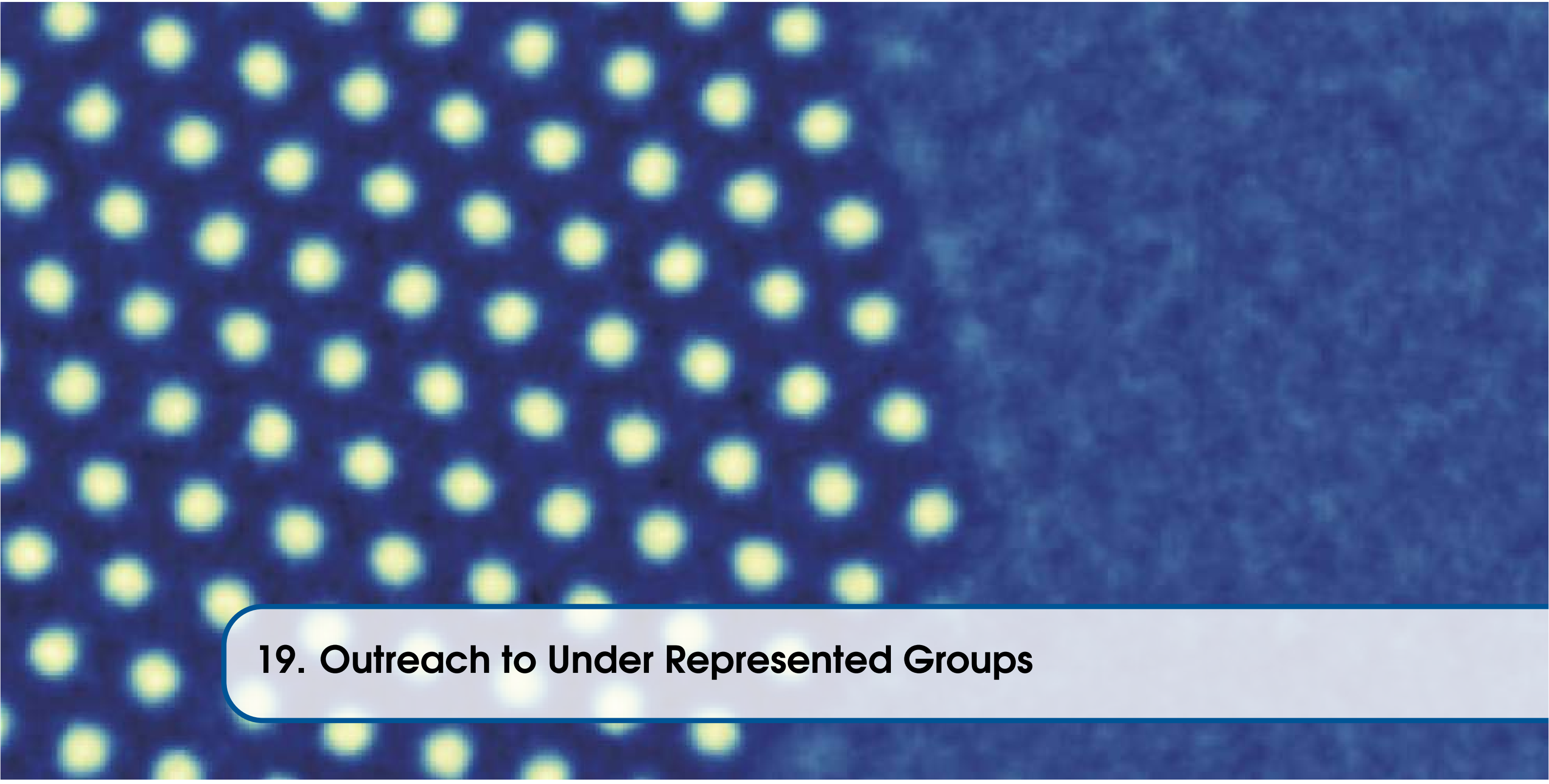
Lead on NSF Midwest Big Data Hub Spoke Proposal

CHiMaD (Lead-PI: **Foster** (UC); Co-PIs: **Agrawal** (NU), **de Pablo** (UC), **Olson** (NU), **Voorhees** (NU) and University of Illinois, Michigan, and Wisconsin) was the lead organization on a three-year proposal to establish a Midwest Spoke on the Integration of Materials Design (IMaD) in the NSF Big Data Spoke program. The proposal was submitted March 2016 and was funded by NSF in February 2017. Also see section 10.7, "Integrative Materials Design: Midwest Big Data Spoke Joint Proposal".

18.4 Future Outlook

In 2017, the CHiMaD Data efforts will concentrate on four primary emphases:

1. Expand CHiMaD resource listings in the CHiMaD/MDF Materials Resource Registry to promote global awareness and discovery of CHiMaD resources.
2. Explore opportunities with NIST and other collaborators in university and industry in one or more targeted pilots on data schema/vocabulary and analytics development for adoption and use in the materials community.
3. Hold 2nd International Data Summit on September 25-26, 2017
4. Play a lead role in Midwest BD Spoke through kickoff meeting, CHiMaD/MDF Materials Resource Registry; and integration of NIST data initiatives in Spoke efforts.



19. Outreach to Under Represented Groups

19.1 Partnership with The University of Chicago Collegiate Scholars Program

Under the leadership of **de Pablo** (UC), CHiMaD partnered with The University of Chicago Collegiate Scholars Program (CCSP) to teach the program's very first *Engineering Core Course* for sophomores during Summer 2016. The University of Chicago Collegiate Scholars Program is a "three year program that aims to prepare talented Chicago Public School students in grades 10-12 for admission and success at the nation's top colleges and universities" *[https://collegiatescholars.uchicago.edu]*. CCSP has a very high rate of success and is especially influential as they follow students through their college studies, as well connect them with a network of previous scholars. Historically the program offers courses on social and basic sciences including humanities, math and chemistry. CHiMaD has brought in its expertise in engineering to introduce and inspire the students into considering applying to 4-year engineering degree programs across the nation.

The 6-week *Engineering Core Course* took place between June 27-August 3, 2016, as two 2-hour sessions each week. It was structured to be a brief introduction to various aspects of engineering and was taught as three modules:

Module 1: Polymers and Composite Materials Module
Instructors: Prof. Juan ***de Pablo*** *(UC), Prof. Paul* ***Nealey*** *(UC), Dr. Xiaoying Liu (UC)*
Teaching Assistants: Ms. Ashley Guo (UC), Mr. Paul Jerger (UC), Mr. Peter Mintun (UC)
This module of the engineering laboratory course focuses on helping students develop skills for the design, execution and optimization of laboratory experiments and analysis and presentation of experimental results through hands-on experience and technical communication practice. The experiments are designed to illustrate the concepts and principles of polymeric and composite materials in the context of real-world applications. Students work in small groups to perform 1-2 experiments per lab session, Figure 19.1. Techniques for measuring material properties and monitoring experimental processes are integrated throughout the course by use of a variety of laboratory instruments and tools.

Module 2: Materials Design and Composites Module
Instructors: Dr. Ricardo Komai (NU)
Teaching Assistants: Dr. Begum Gulsoy (NU), Dr. Andrea Jokisaari (NU), Mr. Shawn Chen, Ms. Ha-Kyung Kwon, Ms. Xiaomi Zhang
This module focuses on the design of materials, specifically composite materials. Students

Figure 19.1: *(Left)* Prof. **de Pablo** (UC) and Module 1 teaching asistants with the CCSP Scholars on the first day of the Summer course. *(Right)* CCSP scholars examining the silly putty they have synthesized during Module 1.

Figure 19.2: *(Top)* Students testing one of the composite samples they have designed during Module 2; Teaching assistant Mr. Chen providing guidance on keeping experimental conditions consistent. *(Bottom)* The class discussing the experimental observations and reasons for failure; Summary of experimental observations for each group, allowing students to evaluate how to improve design strategies in the future.

learn the fundamentals of materials science and engineering including: material types, properties, design of experiments, design of materials, fracture/failure analysis. The module culminates in the second week with a two-session project involving the design of structural composites using the principles observed in the first week. Students prototype multiple design candidates and evaluate which will have superior performance, Figure 19.2.

Module 3: Characterization and Image Processing Module

Instructors: Dr. Begum Gulsoy (NU)
Teaching Assistants: Dr. Andrea Jokisaari (NU), Dr. Ricardo Komai (NU)

This module aims to be an introduction to materials characterization, an important step in materials design and verification. During this module, methods discussed focus on definition of scientific images and 2D image processing with brief examples of 3D data analysis. Students are introduced to images, the difference in perception of images between a human and a computer, what makes scientific images different from everyday photos and how to characterize and interpret scientific images and materials data. The students work in small groups to conduct a serial-sectioning experiment, and perform image analysis. Most of the image analysis is applied using the open software "FIJI", to which students will be briefly introduced to during class. The students explore the software it using both the images they have collected and real scientific images which will be provided by CHiMaD researchers.

Summary and Future Outlook

Overall, the feedback from the students as well as the anonymous feedback they've provided through the post-class survey conducted by CCSP was very positive. The post-class survey showed 75% agree that the course:

- Further increased my interest in STEM
- Made me want to take more STEM courses
- Encouraged me to major in a STEM field
- Expanded my knowledge of the subject

These results, along with individual feedback we have received directly from students at the conclusion of the program, gives us confidence that this was a successful effort and CHiMaD aims to offer the *Engineering Core Course* again in Summer of 2017.

19.2 Partnership with NU-MRSEC Summer REU Program

The Northwestern University Materials Research Science & Engineering Center (NU-MRSEC), under the directorship of Mark **Hersam** (NU), leads a highly regarded 9-week summer research experience for undergraduates (REU). The students who join the program are provided with a stipend, as well as their travel and accommodation expenses. All students are all expected to attend bi-weekly meetings, write regular update reports, a final technical report as well as give a 15-minute oral presentation on their summer research at the end of the 9-week period. The Northwestern leads for the summer program were Aleta Hagman (NU) and Kathleen Stair (NU). In Summer 2016 CHiMaD sponsored Samuel Cabrera of University of California, Irvine (UCI) to join the program under the mentorship of Dr. Ricardo Komai (NU) to work on the project *Prototyping Alloys Designed for Additive Manufacturing* as a part of **Olson** (NU) research group. Cabrera was a senior student majoring in Mechanical Engineering with a minor in Materials Science and Engineering and expected graduation in June 2017 and part of the UC Irvine California Alliance for Minority Participation (CAMP) program.

Printing Alloy Validation –S. Cabrera
(NSF-MRSEC REU; Advisor Dr. R. Komai)

- Co
- Steel
- Ti

Figure 19.3: Compositions designed from MSE 390 regarding a 3D printed Cobalt, Steel, and Titanium alloy were prototyped by CHiMaD REU student Samuel Cabrera (UCI). Alloy prototypes were then heat treated and examined for 3D printing feasibility.

Project Overview: Prototyping Alloys Designed for Additive Manufacturing

During Spring 2016 of Prof. **Olson**'s *MSE 390: Materials Design* course at Northwestern University, three computationally designed alloys for additive manufacturing were proposed: Precipitation Hardened Steel, TRIP Titanium, and Cobalt superalloy. With the increasing relevance of materials produced by Additive Manufacturing, Cabrera (UCI) prototyped each alloy composition through use of an Arc Melter(QuesTek Innovations LLC). These prototypes were then analyzed by optical and scanning electron microscopy with energy dispersive x-ray spectroscopy for phase composition and microstructural features, Figure 19.3. Dendrite segregation profiles were calculation using an Integrated Computational Materials Engineering (ICME) framework and the tool Thermo-Calc. These profiles were then used to predict and validate homogenization treatments of the materials and were performed. Future work includes the corresponding aging treatments of these alloys and further study for precipitation kinetics.

Summary and Future Outlook

The summer project was designed by Komai (NU) and **Olson** (NU) to provide Cabrera experience with both experimental and computational techniques such as:

- Experimental: Arc Melting, Heat Treatments, Optical Microscopy, Scanning Electron Microscopy (SEM), Energy-dispersive X-Ray Spectroscopy (EDS)
- Computational: ThermoCalc

To prepare for the program Cabrera was able to virtually join the 32^{nd} SRG Meeting broadcast in Spring 2016 which provided him with a high-level overview of the subject. At the successful conclusion of the program, Cabrera's work was accepted as a poster presentation to two conferences. CHiMaD and CAMP program together agreed to support his travel and accommodation expenses for the conference. Cabrera applied to several universities, with a focus on pursuing graduate studies in both Mechanical Engineering and Materials Science and Engineering, the latter being partially influenced by his positive experience during the REU program.

CHiMaD plans to partner again with NU-MRSEC REU program for Summer 2017, offering the experience to other undergraduate students interested in learning about and working with materials design concepts. On that note, in 2017, *Materials Design* was explicitly added to the NU-MRSEC REU application website as a separate interest students

Figure 19.4: Sossina Haile (NU) was invited to TMS Summit on Diversity in the Minerals, Metals, and Materials Professions (DMMM2) as a presenter, where the overarching theme of the Summit concentrated on *strategies for increasing underrepresented minority (URM) engagement in the STEM professions*

can indicate.

19.3 Support for & Contribution to TMS Diversity Summit

The Minerals, Metals, and Materials Society (TMS) organized its first *Summit on Diversity in the Minerals, Metals, and Materials Professions (DMMM)* in 2014. Upon the success of the first Summit, TMS organized a second Summit on July 25-26, 2016 at Northwestern University, where CHiMaD acted as the local point-of-contact for the organization providing both monetary and logistics support to the Summit. The 2016 Summit concentrated on the following themes identified during the 2014 Summit, which align with the goals of CHiMaD's outreach to underrepresented groups:

- Strategies for increasing underrepresented minority (URM) engagement in the STEM professions
- Best practices for building a welcoming and inclusive workplace culture
- Addressing factors behind the self-induced glass ceiling and supporting new pathways to career fulfillment

In line with the themes, CHiMaD lead the TMS invitation to Northwestern University, Department of Materials Science and Engineering faculty Sossina Haile (NU) to be a presenter at the *Pipeline Session on Problems, Recommendations and Impact of Workforce Diversity*, Figure 19.4. Haile (NU) was invited to the session due to her active involvement and interest in improving the STEM involvement of underrepresented groups both prior to joining Northwestern as well as after. CHiMaD associate director Begum Gulsoy (NU) was invited by TMS to chair the *Early Career Breakout Session*, where the panelists of the session included Alexis Lewis (NSF), Ellen Cerreta (Los Alamos National Laboratory) and Svetlana Sukhisvili (Texas A & M University). More information for the Summit along with the final agenda can be found on TMS website [*http://www.tms.org/meetings/2016/diversity2016*]

The TMS *Summit on Diversity in the Minerals, Metals, and Materials Professions (DMMM)* is a bi-annual Summit, the next one of which is expected to be organized in 2018. CHiMaD aims to return to the Summit as a supporter and, if invited by organizers, have further programmatic involvement once again.

19.4 Interactions with Fayetteville State University

Through a CHiMaD-ThermoCalc initiative, Fayetteville State University (FSU) was awarded a 3-year license to the ASM Materials Genome Toolkit in 2015. The software and databases included in the ASM Materials Genome Toolkit were fully-installed by Fayetteville State University in 2016, under the leadership of CHiMaD principal investigator Alexander **Umantsev**. Mr. Furaha, a CHiMaD undergraduate student working with **Umantsev** was sponsored to attend the Materials Genome Toolkit and Materials Design Training that took place at Carnegie Mellon University on July 6-8 2016. For more information on the ASM Materials Genome Toolkit and the accompanying Materials Genome Toolkit and Materials Design Training please see Section 16.1.

VI

Other

20. Honors & Awards

Awards received by CHiMaD PIs in 2016

Wei Chen, *Northwestern University*
2016 Best Paper Award, 42th ASME Design Automation Conference for paper Yu, S., Zhang, Y., Wang, C., Lee, W-K, Dong, B., Sun, C., Odom, T., and Chen, W., "Characterization and Design of Functional Quasi-Random Nanostructured Materials using Spectral Density Function"

Alok Choudhary, *Northwestern University*
2016 BITS Pilani Distinguished Alumni Award, Birla Institute of Technology &Science, India

Juan De Pablo, *University of Chicago*
Fellow, National Academy of Engineering
Dupont Science Excellence Medal
Chair, Condensed Matter and Materials Research Committee, National Research Council
PPEPPD Plenary Speaker, Porto, Portugal
Chair, Advisory Committee, Mathematical and Physical Sciences Division, National Science Foundation

Mark Hersam, *Northwestern University*
U.S. Science Envoy, U.S. Government
Institute of Electrical and Electronics Engineers (IEEE) Fellow, IEEE Organization

Sinan Keten, *Northwestern University*
APS Fellow, American Physical Society
ONR Director of Research Early Career Award, Office of Naval Research

Heinrich Jaeger, *University of Chicago*
2016 Award for Excellence in Graduate Teaching, University of Chicago

Tobin Marks, *Northwestern University*
2016 Chinese Academy of Sciences President's International Distinguished Scientist (Einstein) Award
2016 Member, U.S. National Academy of Inventors
2016 Tannas Award in Materials Science, University of California, Los Angeles
2016 Eminent Scientist Award, American Chemical Society Undergraduate Program
2016 Honorary Professor, Chinese Academy of Sciences, Dalian Institute of Chemical Physics
2016 Doctor of Science Honoris Causa, Technical University of Munich
2016 Munib and Angela Masri Distinguished Lecturer, American University of Beirut
2016 ECS Distinguished Faculty Lecturer, University of Texas Dallas
2016 Science at the Cutting Edge Lecturer, Michigan State University
2016 McElvain Academic Lecturer, University of Wisconsin Madison
2016 Zhang Dayu Lecturer, Chinese Academy of Sciences Institute of Chemical Physics

Sidney Nagel, *University of Chicago*
2016 Fritz London Lecture, Duke University
2016 Hoxton Lecture, University of Virginia
2016 Ryerson Lecture, University of Chicago

Paul Nealey, *University of Chicago*
Semiconductor Research Corporation University Researcher Award, Semiconductor Industry Association

Monica Olvera de la Cruz, *Northwestern University*
Polymer Physics Prize, American Physical Society

David Seidman, *Northwestern University*
2016 Fellow of the Inaugural Class, International Field Emission Society (for atom-probe tomography)

Steven Sibener, *University of Chicago*
2016 Elected Fellow, American Vacuum Society
2016 Elected Fellow, American Chemical Society

Matthew Tirrell, *University of Chicago*
2016 Covestro Lectures, University of Pittsburgh
2016 Wilhelm Lectures, Princeton University

Alexander Umantsev, *Fayetteville State University*
2015-2016 Fulbright U.S. Scholar Award, J. William Fulbright Foreign Scholarship Board
Travel Award, Kumamoto University, Japan

Peter Voorhees, *Northwestern University*
Member, American Academy of Arts and Sciences

Awards received by CHiMaD Students and Postdoctoral Researchers in 2016

Jennifer Bennett, *Cao Research Group, Northwestern University*
2016 Guy E. Boudreau Scholarship, Additive Manufacturing Users Group

Hadallia Bergeron, *Hersam Research Group, Northwestern University*
NSF Graduate Research Fellowship, National Science Foundation
NSERC Postgraduate Scholarship, Natural Sciences and Engineering Research Council, Canada

Ding-Wen (Tony) Chung, *Seidman/Dunand Research Groups, Northwestern University*
Institute of Sustainability and Energy Cluster Fellowship, Northwestern University

Ha-Kyung Kwon, *Olvera de la Cruz Research Group, Northwestern University*
International Institute for Nanotechnology Outstanding Researcher Award, Northwestern University

Andrea Jokissari, *Heinonen Research Group, Argonne National Laboratory*
Editor's Choice for paper Jokisaari, A. M., Voorhees P. W., Guyer, J.E., Warren J., Heinonen, O.G., "Benchmark problems for numerical implementations of phase field models" Comp. Mater. Science. 126 139-151 (2017) [DOI: 10.1016/commatsci.2016.09.022]

Bobby Sinko, *Keten Research Group, Northwestern University*
National Defence Science & Engineering Graduate Fellowship, Department of Defense

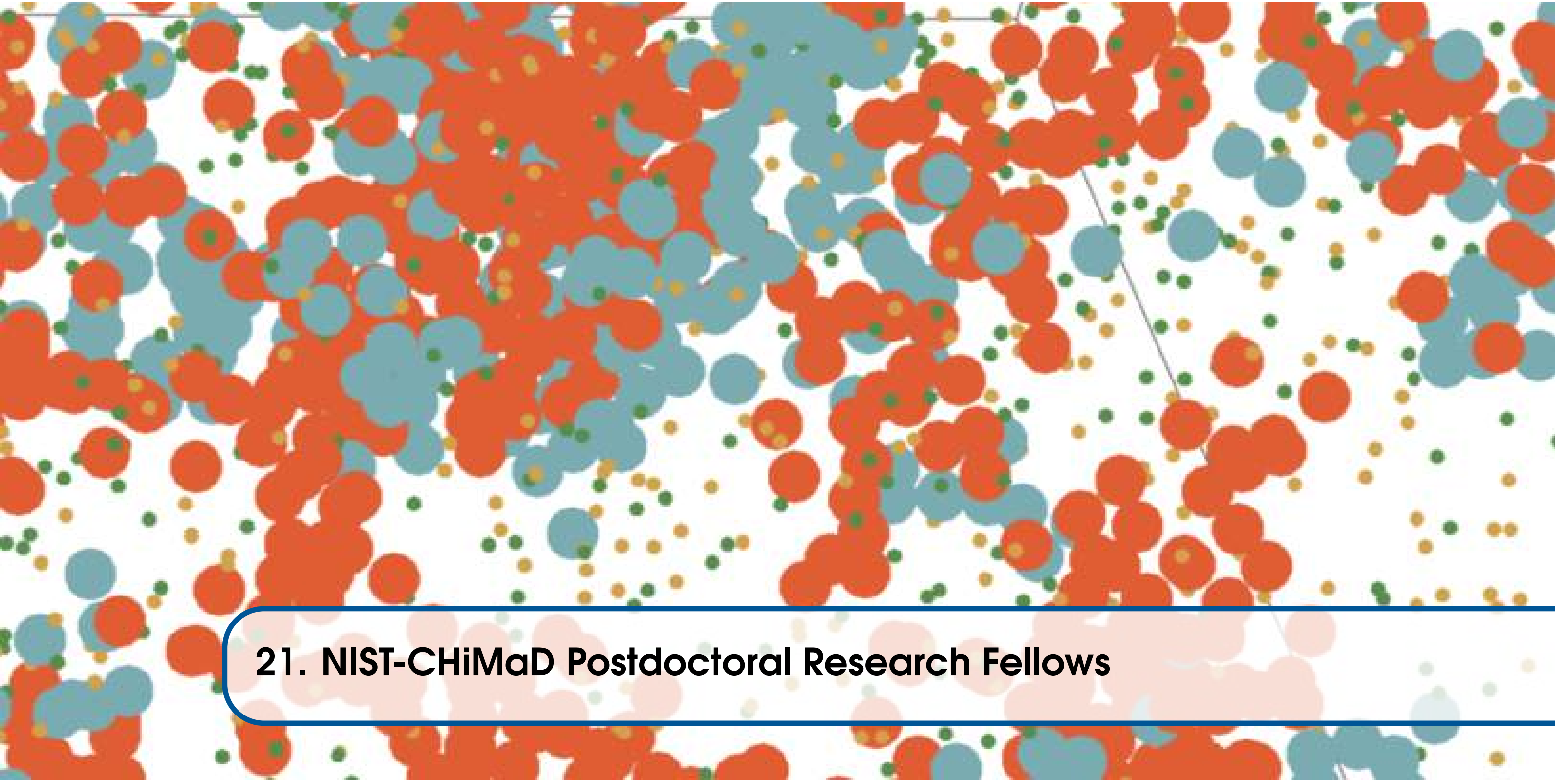
Jake Song, *Keten Research Group, Northwestern University*
2nd Place, NDConnect 2016 Undergraduate Research Competition, University of Notre Dame

Johnathan Raybin, *Sibener Research Group, University of Chicago*
Charles H. Viol Fellowship

Matthew Peters, *Voorhees Research Group, Northwestern University*
Larry Kaufman Scholarship, The Minerals, Metals and Materials Society Foundation

Jeffrey Ting, *Tirrell Research Group, University of Chicago*
2016 Sigma Xi Charles and Dorothy Andrew Bird Award, Sigma Xi Society
University of Minnesota Doctoral Dissertation Fellowship

Wenjie Xia, *Keten Research Group, Northwestern University*
APS Padden Symposium Finalist, American Physical Society
Best paper award, Midwest Workshop on Mechanics and Materials, Northwestern University
Chinese Government Award for Outstanding Students Abroad, China Scholarship Council, China



21. NIST-CHiMaD Postdoctoral Research Fellows

Marat Andreev (UC/NIST)

Soft Matter Design Based on Charge Complexation
Supervisors: Juan De Pablo (UC), Jack Douglas (NIST)
Other CHiMaD Collaborators: Matthew Tirrell (UC)
Other NIST Collaborators: Vivek Prabhu (NIST), Debra Audus (NIST), Alexandros Chremos (NIST), Jack Douglas (NIST)

Bio *Dr. Andreev was born in Siberia, Russia. He received his B.Sc and M.Sc degrees from Novosibirsk State University. In 2009 he joined Professor Jay Schieber's research group at Illinois Institute of Technology and was awarded his Ph.D. in December 2014. He then joined the* ***De Pablo*** *group at University of Chicago as postdoctoral researcher; in 2015 and 2016 he was awarded a NIST-CHiMaD postdoctoral research fellowship.*

21.1 Research Accomplishments

Dr. Andreev's research concentrates on polyelectrolyte complexation. In brief, it is entropically beneficial for oppositely charged polyelectrolytes to release counter-ions and form polymer rich regions by electrostatic attraction. Primarily, he developed the coarse-grain molecular dynamics approach to the problem and used it to study a number of cases computationally. Additionally, the implementation uses GPUs for numerical acceleration.

For homopolymers, the complexation leads to a phase separation. Here, the composition of polymer rich phase, known as coacervate, and supernatant phase is a subject of research attention. Last year, he was able to estimate polymer and exact salt composition for a number of molecular weights and overall salt compositions in the mixture of PAA/PDMAEMA. He summarized results in a phase diagram and got a qualitative agreement with experimental data by Spruijt el al. (Macromolecules 2012). This year he focused on refining the phase diagram. Firstly, the iterative method for equilibrating chemical potentials and pressure of both phases was implemented. Here, the Widom insertion technique

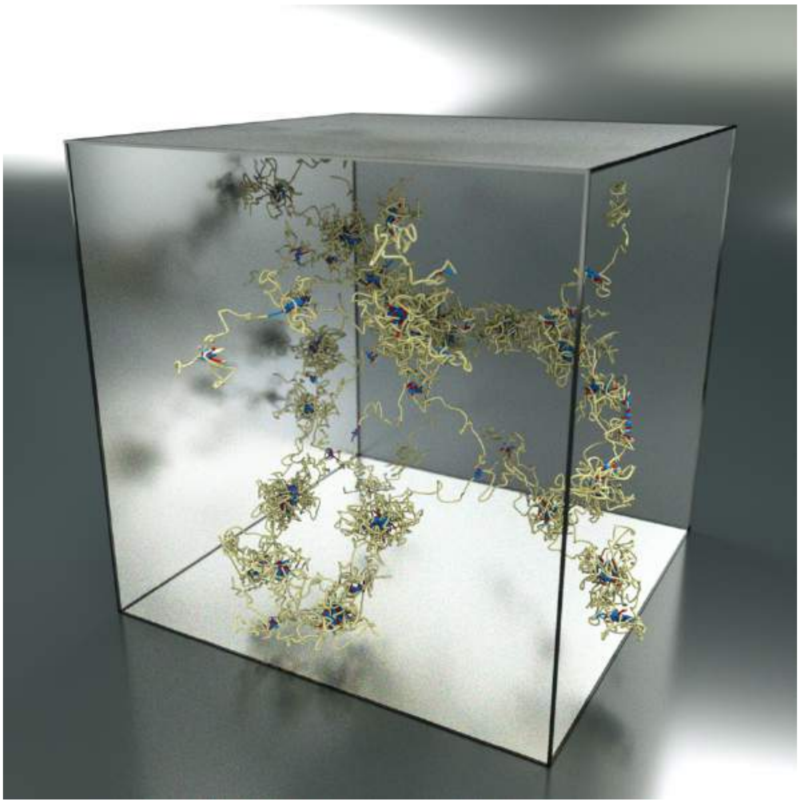


Figure 21.1: Snapshot from MD simulation of triblock copolyelectrolytes assembly(40-200-40 ABA triblock at 0.36$wt\%$ polymer concentration). Charged end-blocks (blue and red) form polyelectrolyte complex cores, while midblocks (yellow) make up a percolating structure, resulting in gel-like material.

allowed for chemical potential calculation. Additionally validations were performed by Gibbs/semi-grandcanonical simulations. Both techniques yield in lower salt concentration in coacervate phase are in good agreement with each other and in qualitative agreement with experimental observations by the **Tirrell** (UC) research group. A publication on results from this research was submitted for publication in ACS Macro Letters.

For copolymers he performed large scale simulations to compliment experimental findings of the **Tirrell** (UC) group at UC and the **Prabhu** (NIST) research group at NIST. This work resulted in a publication in Nature Communications [25.24] and detailed description is provided below. Additionally he contributed to a work of **Audus** (NIST) and Srivastava (UC) to study micelle formation in case of diblock copolyelectrolytes. A manuscript on that work is prepared for submission to publication.

Dynamics of homopolymer coacervate was the focus of Dr. Andreev's collaboration with **Chremos** (NIST) and **Douglas** (NIST). Previously he showed that his model doesn't capture dependence of diffusion coefficients and relaxation times on salt concentration. Based on previous studies of the **Douglas** (NIST) group, they modified cohesive interaction to mimic solvation effects and were able to get positive response in dynamical properties. For simplicity they aimed to reproduce available ion diffusion data. A publication is in preparation.

21.2 Collaborations

21.2.1 NIST Collaborations

Micelle Formation in Diblock Copolyelectrolytes

*Marat Andreev (UC-NIST), Debbie **Audus** (NIST)*

This collaboration investigated the formation of micelles by polyelectrolyte diblocks where the primary research targets were equilibrium micelle size and aggregation number. Extensive simulations of self-assembly by Andreev (UC-NIST) were aided by *umbrella* sampling technique calculation of single micelles. Effects of polymer architecture and molecular weight were explored in detail by thermodynamical integration calculation and scaling theory of **Audus** (NIST).

Dynamics of Homopolymer Coacervate

*Marat Andreev (UC-NIST), Alex **Chremos** (NIST), Jack **Douglas** (NIST)*

During this collaboration, dynamics of homopolymer coacervate were investigated. To mimic solvation effects, Andreev modified the cohesive interactions in the model he had developed, using the data from **Douglas** (NIST) group at NIST and was able to obtain positive dynamic properties.

21.3 Publications and Presentations

1 Number of CHiMaD-supported publications in 2016. Please see chapter 25 for details [25.23].

7 Number of presentations on CHiMaD supported research in 2016, please see section 24.6 for the complete list.

Nana Ofori-Opoku (NU/NIST)

Phase-Field Methods

Supervisors: Peter Voorhees (NU), James Warren (NIST)

Other NIST Collaborators: Jonathan Guyer (NIST), Supriyo Ghosh (NIST)

Bio *Dr. Ofori-Opoku holds a Ph.D. from the Materials Science and Engineering Department, McMaster University. While completing his Ph.D., he held multiple appointments as visiting researcher at TKK Aalto University and VTT Technical Research Centre in Finland. Before joining CHiMaD as a NIST-CHiMaD Postdoctoral Research Fellow, he was a postdoctoral fellowship at McGill University working on recrystallization kinetics and microstructure development for nanoscale devices using continuum and atomistic models. His research interests combine computational materials science and condensed matter physics, with emphasis on multi-scale modeling of non-equilibrium materials phenomena and microstructure evolution.*

21.4 Research Accomplishments

A phase-field crystal model, a continuum atomistic methodology, has been investigated and found to be well suited for describing the solidification microstructures associated with highly anisotropic and faceted interfaces. We have found however that the model is limited, particularly in describing microstructural features on length scales of interest. Due to this length scale limitation, we have developed, through coarse-grained approaches, a phase-field type description of the model. The resultant model operates on larger length scales, however it retains some salient atomistic features of the original formulation. These features include the description of the underlying crystal lattice of interest through reciprocal lattice vectors. Using 1D calculations, Dr. Ofori-Opoku has performed simulations investigating the equilibrium properties of solid-liquid interfaces. It was found that by measuring surface energetics and calculating equilibrium shapes via Wulff constructions, that this larger length scale model is well equipped in describing anisotropic surfaces. It should be noted that the self-consistently derived coarse-grained model has many of the same features of several phenomenological models and theories postulated to describe surfaces through such variables as the height function. A representative figure demonstrating the properties of the model is shown in Figure 21.2. As a function of the system temperature, the surface energy (polar form) and the resultant Wulff construction are shown, where the beginning of the emergence of the anisotropic shape can be observed.

21.5 Collaborations

21.5.1 NIST Collaborations

On the Primary Spacing of Laser Deposited Dendrites in Ni-Nb Alloys

Nana Ofori-Opoku (NU-NIST), Supriyo Ghosh (NIST), Jonathan ***Guyer*** *(NIST)*

A phase-field method is used to investigate the microstructure features of additive manufactured Ni-Nb alloys.

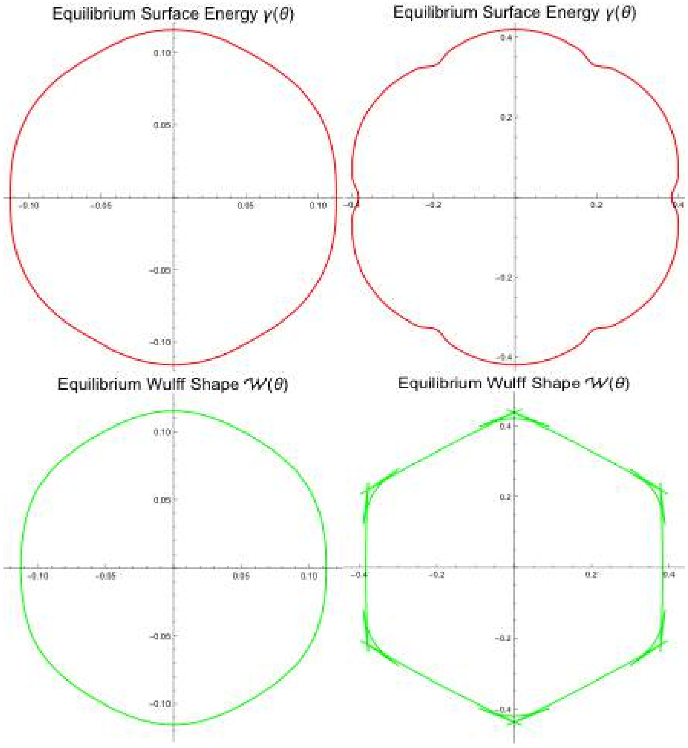


Figure 21.2: Equilibrium Surface energy and Wulff Shape in polar coordinates. System temperature decreases from left to right, with the top row showing the surface energy while the bottom row shows the Wulff shape construction. Note the emerging cusps (rounded) in the surface energy and the accompanying emergence of ears in the Wulff construction.

21.5.2 External Collaborations

Multi-Order Parameter Phase-Field Model From a Grand Potential
Nana Ofori-Opoku (NU-NIST), Nikolas Provatas (McGill University)
Quantitative phase-field method is used to study the second phase nucleation and growth using self-consistent coarse-grained fluctuations.

Phase-Field Crystal Modeling of Graphene Growth
Nana Ofori-Opoku (NU-NIST), Nikolas Provatas (McGill University)
An alloy phase-field crystal model is developed to investigate the dendritic growth of graphene on substrates in collaboration with Elder (McGill University) and Provatas (McGill University).

Phase Field Modeling of Thermal Spray Coatings in W-C system
Nana Ofori-Opoku (NU-NIST), Nikolas Provatas (McGill University), Anssi Laukkanen (VTT Technical Research Centre of Finland)
Consulting on developing a phase field model and numerical techniques to describe the rapid solidification in spray coatings.

Solidification in the Presence of Flow
Nana Ofori-Opoku (NU-NIST), Arvind Baskaran (Brandeis University)
his collaboration focuses on developing an effective phase field model, derived from the phase field crystal model, with hydrodynamic interactions to apply to modeling of dendrite fragmentation during solidification.

Quantitative Modeling Using Phase-Field Crystal
Nana Ofori-Opoku (NU-NIST), David Simeone (CEA-CNRS-ECP), Laurence Luneville (CEA-CNRS-ECP), Vassilis Pontikis (CEA)
This collaboration focuses on developing formulations for the quantitative description of Ag-Cu system using phase-field crystal.

21.6 Publications and Presentations

1 Number of CHiMaD-supported publications in 2016. Please see chapter 25 for details [25.26].

4 Number of presentations on CHiMaD supported research in 2016, please see section 24.6 for the complete list.

Peisheng Wang (NU/NIST)

Precipitation Strengthened Alloys

Supervisors: Gregory Olson (NU), Ursula Kattner (NIST), Carelyn Campbell (NIST), Eric Lass (NIST)

Bio *Dr. Wang's main research interest lies in thermodynamic calculations (CALPHAD). He received his Ph.D. in 2012 from Central South University, China for experimental determination of Mg phase diagram and thermodynamic calculations. He was then a postdoctoral researcher at TU Clausthal, Germany between 2012-2014. During his postdoctoral work he was interested in Heterogeneous Nucleation and Microstructure Formation of Al-Cu-Ni alloys and a new function to describe the Gibbs energy of liquid phase. In 2015 he was awareded a NIST-CHiMaD Postdoctoral Research Fellowship to futher CALPHAD methods under Precipitation-Strengthened Alloys use-case group.*

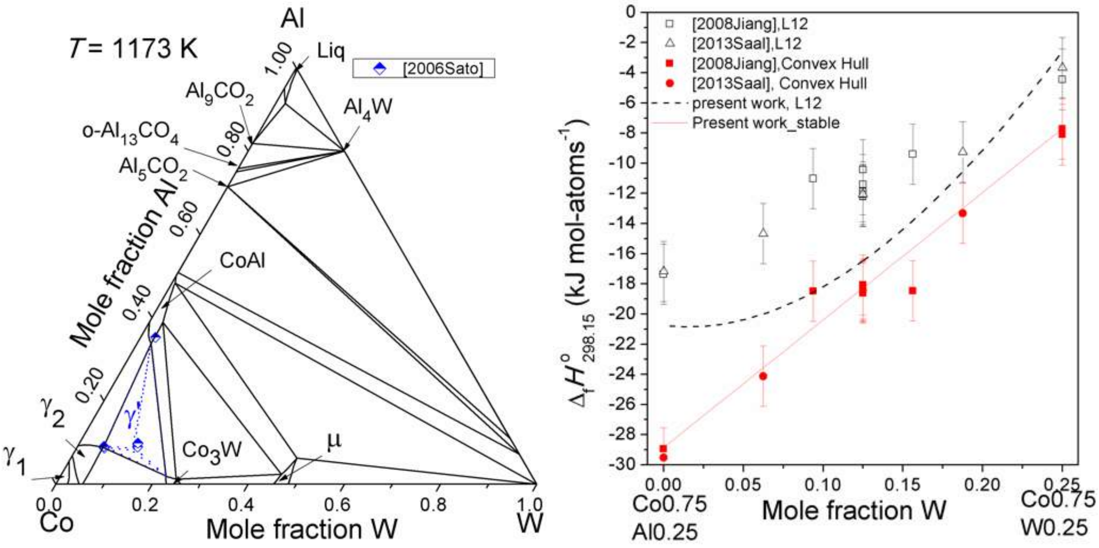


Figure 21.3: From left to right: (A) Calculated isothermal section at 1173^oK with calculated metastable γ' phase equilibria superimposed. (B) Calculated enthalpy of formation of the $\gamma' L1_2$ phase and enthalpy of formation for the stable status compared with DFT results from literature DFT error bars were assessed as $2kJ$.

21.7 Research Accomplishments

Efforts to establish a multi-component thermodynamic database (CALPHAD), for the design of Co-based superalloys, continue to progress through the efforts of Wang (NU-NIST), Xiong (University of Pittsburgh) and **Olson** (NU). In addition to the primary focus of the Precipitation Strengthened Alloys use-case group, Cr, Re and Ru was added into the current database. An 9-component thermodynamic database Co-Al-W-Ni-Ti-Ta-Cr-Re-Ru system is now deliverable. The Al-Ni, Co-W, Co-Re, Ni-Re, Co-Ta, Co-Al-W, Co-Al-Ni, Co-Al-Ti, Al-Ni-W, Co-Ni-W and Co-Al-W-Ni systems were reviewed and optimized by cooperating density functional theory (DFT) calculations during 2016.

The predicted calculation of multi-component system (Co-Al-W-Ni-Ta-Ti) using current database is consistent with experimental data, which is a significant improvement compared to the calculation using available commercial thermodynamic databases. One of the representative accomplishments is the optimization for Co-Al-W system, as shown in Figure 21.3A-B.

In the next year, Dr. Wang will focus his research on the refinement of the thermodynamic database: (1) Experimental studies and thermodynamics assessments of the Co-Cr-X (X = Al, Ni, Ta, Ti, W); (2) Thermodynamic assessment of the Co-Al-Cr-X and Co-Al-W-Ni-X systems.

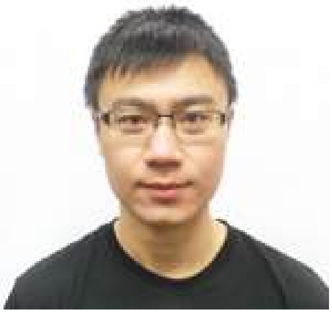
21.8 Collaborations

21.8.1 NIST Collaborations

Thermodynamic Databases

Peisheng Wang (NU-NIST), Ursula ***Kattner*** *(NIST), Carelyn* ***Campbell*** *(NIST), Eric* ***Lass*** *(NIST)*

Dr. Wang developed the thermodynamic database using experimental data produced by NIST researchers, **Kattner**, **Campbell** and **Lass**. He also contributed to the NIST thermodynamic database for Co-based superalloys; this new database was used for new alloy composition screening and materials design, as well as kinetic simulations.



Wenjie Xia (NU/NIST)

Polymer Matrix Materials

Supervisors: Sinan Keten (NU), Frederick Phelan (NIST), Jack Douglas (NIST)

Bio Dr. Wenjie Xia finished his Ph.D. from the Department of Civil and Environmental Engineering at Northwestern University in 2016. During his doctoral study, his research focused on computational mechanics and multi-scale modeling of polymer nanomaterials. After his Ph.D., he was awarded a NIST-CHiMaD Postdoctoral Fellowship to develop scale-bridging techniques and computational models for investigation of soft matters. He has received the Water P. Murphy Fellowship and been selected as the finalist for the American Physical Society Frank J. Padden Jr Award for excellence in graduate polymer research. He has also received the Chinese government award for outstanding students abroad.

Dr. Xia's research mainly focuses on development of scale-bridging computational techniques, such as coarse-grained (CG) modeling approach as illustrated in Figure 21.4, to facilitate computational design of polymeric materials. Dr. Xia also has employed the developed models to investigate polymeric nanostructured systems, such as thin films and nanocomposites, and gain fundamental understanding of interfacial confinement effects on polymeric systems for materials design and development.

Previous coarse-graining techniques remain questionable due to its inability to accurately reproduce atomistic polymer dynamics across different temperature regimes. While there has been intense activity in this field to solve this fundamental problem, a systematic solution has yet been developed. Though collaboration with **Phelan** (NIST) and **Douglas** (NIST), Dr. Xia has addressed this critical lack of progress in the field through a novel CG modeling strategy, namely the energy renormalizing approach. The established approach can capture the dynamics of the representative polymer system over a wide range of temperatures at extended time and length scales.

This collaborative research has uncovered the intrinsic difference between the reduced order model (i.e., CG model) and atomistic model of polymer, which is the temperature scaling of activation energy and configurational entropy. The established CG modeling framework through Dr. Xia's efforts is salient not only for polymers, but also for many other classes of glass, such as biomolecules, metallic glasses, and even simple molecular liquids, where cooperative dynamics and glass-forming process occur upon supercooling. Moreover, the approach provides computation-based materials-by-design strategy to develop advanced glass-forming materials with tunable properties, such as fragility, relaxation dynamics and activation energy.

21.9 Collaborations

21.9.1 CHiMaD Collaborations

Understanding Mechanical Interphase in Nanoscale Polymer Thin Films

*Wenjie Xia (NU-NIST), Sinan **Keten** (NU), Catherine **Brinson** (NU)*

This collaboration focuses on understanding the nanoscale interphase formed near the substrate or filler interphase in polymeric systems. Utilizing the coarse-grained molecular

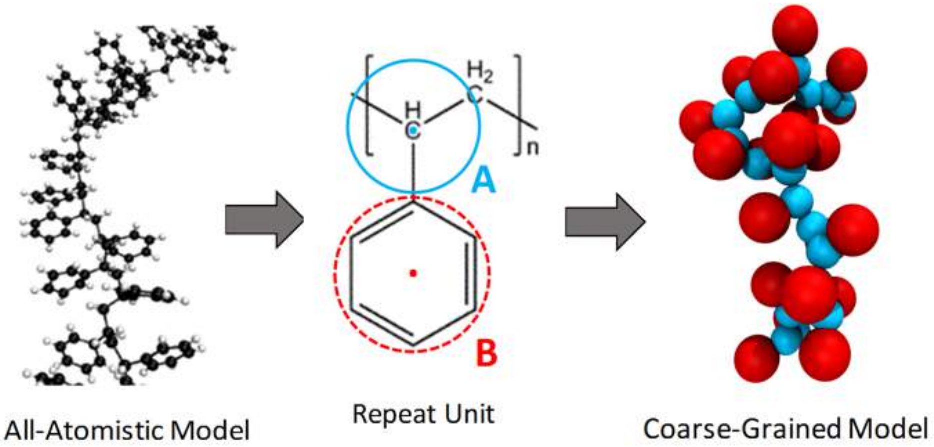


Figure 21.4: The atomistically informed coarse-grained model of polystyrene, showing the mapping from (left) all-atomistic (AA) model to (right) coarse-grained (CG) model. (Middle) For each repeat unit, backbone type *"A"* CG bead is centered on the alkyl carbon bonded to phenyl ring. Side chain type *"B"* CG bead is located at the center mass of the phenyl ring.

dynamics simulations of nanoindentation, this research reveals that there exists local stiffness gradient in the polymer films with the magnitude of local stiffness decreasing from the interface to the interior region and free surfaces.

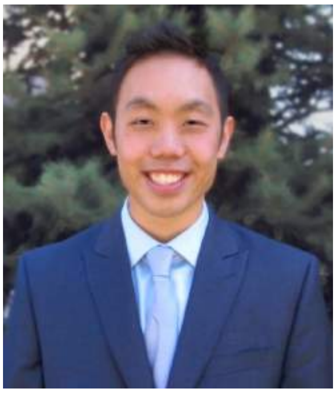
21.9.2 NIST Collaborations

Temperature Transferable Coarse-graining Models for Polymer Dynamics
Wenjie Xia (NU-NIST), Frederick ***Phelan*** *(NIST), Jack* ***Douglas*** *(NIST)*
This collaboration focuses on development of scale-bridging technique for simulating polymer at extended time and length scales. The developed coarse-grained model through a novel approach, called the energy renormalizing approach, can capture the dynamics of the representative polymer system over a wide range of temperatures.

21.10 Publications and Presentations

2 Number of CHiMaD-supported publications in 2016. Please see chapter 25 for details [25.6, 25.7].

2 Number of presentations on CHiMaD supported research in 2016, please see section 24.6 for the complete list.



Jeffrey Ting (UC/NIST)

Soft Matter Design Based on Charge Complexation

Supervisors: Matthew Tirrell (UC), Frederick Phelan (NIST), Jack Douglas (NIST)

Bio *Dr. Ting received his B.S. degree in chemical engineering at the University of Texas in 2011, where he conducted research for Dr. C. Grant Willson. He joined the research groups of Profs. Frank S. Bates and Theresa M. Reineke at the University of Minnesota and earned his Ph.D. in chemical engineering in 2016. During his graduate studies, Dr. Ting was a recipient of the NSF Graduate Research Fellowship and Minnesota Dissertation Doctoral Fellowship, which supported his work in developing new polymer formulations for controlled oral drug delivery. In September 2016, he joined the Tirrell group at the University of Chicago as a NIST-CHiMaD postdoctoral fellow, where his focus will be on exploring structure-property relationships and assembly features of polyelectrolyte complexes.*

21.11 Research Accomplishments

Polyelectrolyte complexes (PECs) can address broad societal needs as key ingredients in advanced biomaterials. These systems are assemblies of oppositely-charged polymers in aqueous solutions, which can be incorporated into various applications to judiciously design multifunctional nanomedicine carriers for tissue engineering, gene therapy, and theranostic probes. Figure 21.5 depicts this general PEC process. My current work involves studying the structural evolution, dynamics, and behavior of designer multiblock polymers as PECs in solution for new biomaterials applications. The goal of this work is to better understand how chain microstructures, properties and hiearchical architectures affect the assembly mechanism and kinetics of entropy-driven PEC formation, which can range from PEC-core micelles to stimuli-responsive hydrogels.

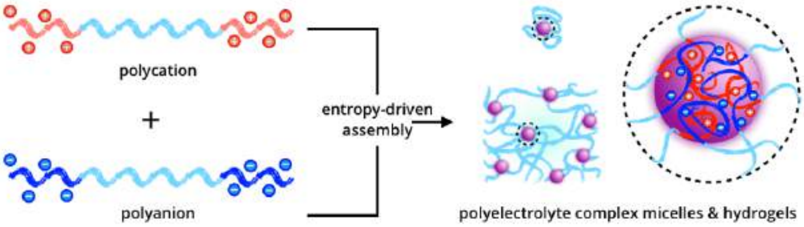


Figure 21.5: Illustration of polyelectrolyte complex (PEC) assembly process from tailorable polycations and polyanions. The effects of new polymer platforms with modular ionic character, molecular architecture, and chemical moieties on resultant mechanical, rheological, and responsive PEC properties will be pursued.

22. CHiMaD Principal Investigators and Staff

22.1 CHiMaD Principal Investigators

Peter Voorhees
CHiMaD Co-Director
Frank C. Engelhart Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Gregory Olson
CHiMaD Co-Director
Walter P. Murphy Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Juan De Pablo
CHiMaD Co-Director
Liew Family Professor in Molecular Engineering
Institute for Molecular Engineering
University of Chicago

Ankit Agrawal
Research Associate Professor
Department of Electrical Engineering and Computer Science
Northwestern University

Micheal Bedyzk
Department Chair and Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Larry Berardinis
Technology Projects Manager, Computational Materials Data (CMD) Network
ASM International

Ida Berglund
Materials Design Engineer
QuesTek Innovations LLC

Catherine Brinson
Jerome B. Cohen Professor of Mechanical Engineering
Associate Dean for Academic and Professional Initiatives
Department of Mechanical Engineering
Northwestern University

Jian Cao
Associate Vice President of Research
Director of Northwestern Initiative for Manufacturing Science and Innovation (NIMSI)
Professor of Mechnical Engineering
Department of Mechanical Engineering
Northwestern University

Wei Chen
Wilson-Cook Professor in Engineering Design
Professor of Mechanical Engineering
Department of Mechanical Engineering
Northwestern University

Alok Choudhary
Henry Isabelle Dever Professor of Electrical Engineering and Computer Science
Department of Electrical Engineering and Computer Science
Northwestern University

Yip-Wah Chung
Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Stephen Davis
Walter P. Murphy Professor of Engineering Sciences and Applied Mathematics
Department of Engineering Sciences and Applied Mathematics
Northwestern University

Dana Frankel
Materials Design Engineer
QuesTek Innovations LLC

Ian Foster
Director, Computation Institute
Professor, Department of Computer Science
Senior Scientist, Mathematics and Computer Science Division
University of Chicago
Argonne National Laboratory

Giulia Galli
Liew Family Professor in Molecular Engineering
Institute for Molecular Engineering
University of Chicago

Olle Heinonen
Strategic Initiative Lead in Computational Chemistry and Materials
Materials Scientist
Fellow, Northwestern-Argonne Institute of Science and Technology
Materials Science and Engineering Division
Argonne National Laboratory

Scott Henry
Director, Content & Knowledge-Based Solutions
ASM International

Mark Hersam
Walter P. Murphy Professor of Materials Science and Engineering
Director, Materials Research Science and Engineering Center (MRSEC)
Department of Materials Science and Engineering
Northwestern University

Clay Houser
Materials Engineer
QuesTek Innovations LLC

Heinrich M. Jaeger
William J. Friedman and Alicia Townsend Professor of Physics
James Franck Institute and Department of Physics
University of Chicago

Sinan Keten
Assistant Professor of Mechanical Engineering
Assistant Professor of Civil and Environmental Engineering
Department of Mechanical Engineering
Department of Civil and Environmental Engineering
Northwestern University

Lincoln Lauhon
Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Wing-Kam Liu
Walter P. Murphy Professor of Mechanical Engineering & Civil and Environmental Engineering
Department of Mechanical Engineering
Department of Civil and Environmental Engineering
Northwestern University

Erik Luijten
Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Engineering Sciences and Applied Mathematics
Northwestern University

Tobin J. Marks
Charles E. and Emma H. Morrison Professor of Chemistry
Professor of Materials Science and Engineering
Vladimir N Ipatieff Professor of Catalytic Chemistry
Department of Chemistry
Northwestern University

Sidney Nagel
Stein-Freiler Distinguished Service Professor
James Franck Institute and Department of Physics
University of Chicago

Paul Nealey
Brady W. Dougan Professor in Molecular Engineering
Institute for Molecular Engineering
University of Chicago

James Saal
Sr. Materials Design Engineer
QuesTek Innovations LLC

Jason Sebastian
Director of Technology
QuesTek Innovations LLC

Kenneth Shull
Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Steven Sibener
Carl William Eisendrath Distinguished Service Professor
Department of Chemistry and The James Frank Institute
University of Chicago

Barry Smith
Senior Computational Mathematician
Senior Fellow, Northwestern-Argonne Institute of Science and Technology
Mathematics and Computer Science Division
Argonne National Laboratory

David Snyder
Sr. Materials Development Engineer
QuesTek Innovations LLC

Matthew Tirrell
Dean and Founding Pritzker Director
Institute for Molecular Engineering
University of Chicago

Monica Olvera de la Cruz
Lawyer Taylor Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Alexander Umantsev
Professor of Physics
Department of Chemistry and Physics
Fayetteville State University

Christopher Wolverton
Professor of Materials Science and Engineering
Department of Materials Science and Engineering
Northwestern University

Luping Yu
Professor of Chemistry
Department of Chemistry
University of Chicago

22.2 CHiMaD Technical Leads

∗ *denotes technical leads who are no longer CHiMaD affiliated*

Emine Begum Gulsoy
CHiMaD Associate Director
Fellow, Northwestern-Argonne Institute of Science and Engineering
Research Associate
Department of Materials Science and Engineering
Northwestern University

Laura Bartolo
CHiMaD Data & Database Efforts Coordinator
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Paul Adler
CHiMaD Metals Processing Facility Manager
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Ricardo Komai∗
CHiMaD Materials Design Expert
Postdoctoral Researcher
Department of Materials Science and Engineering
Northwestern University

22.3 CHiMaD Administrative Staff

∗ *denotes administrative staff members who are no longer CHiMaD affiliated*

Deneen Marie Bryce
Business Administrator
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Sandra Marijan
Executive Assistant
Institute for Molecular Engineering
University of Chicago

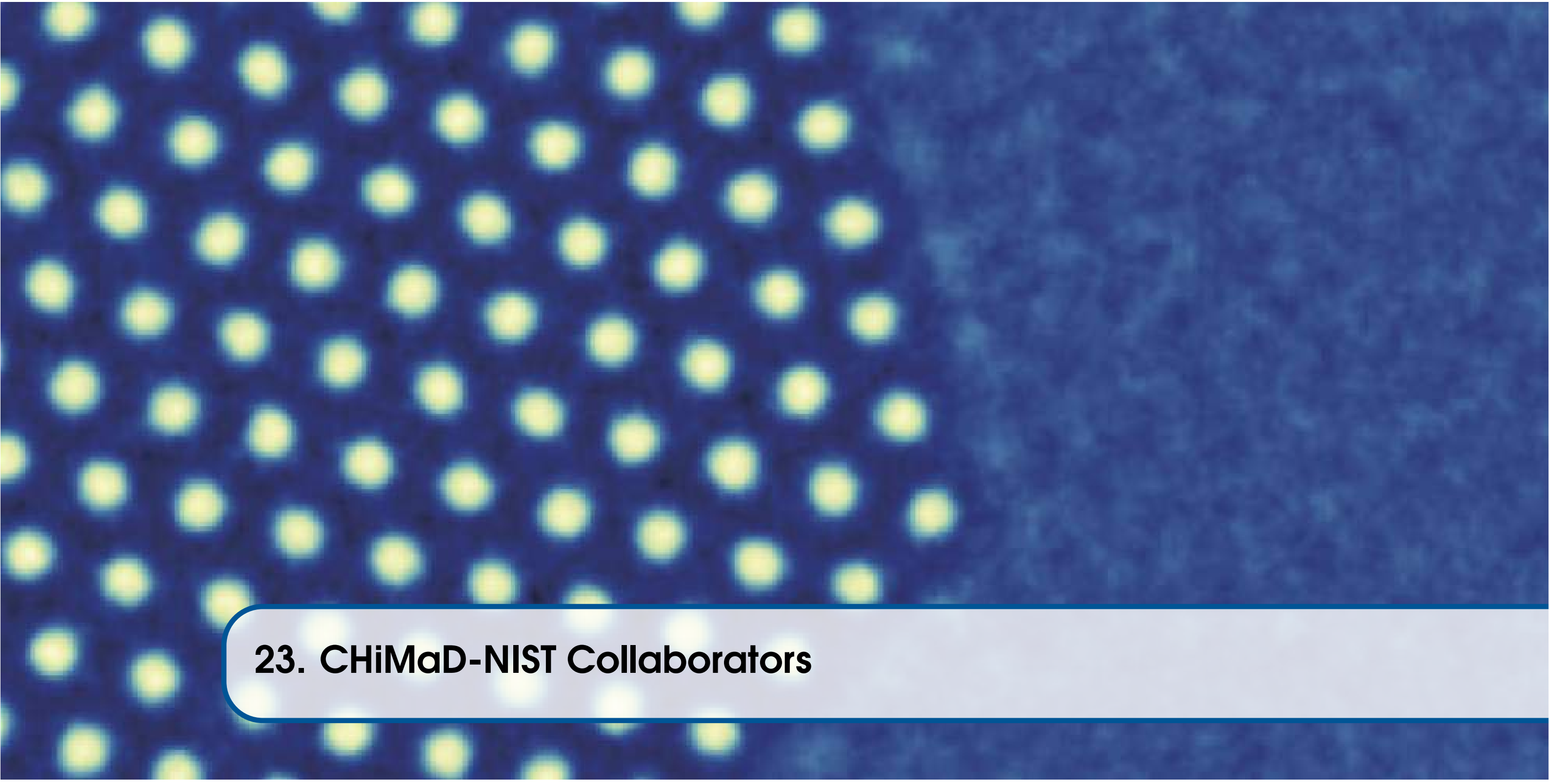
Kathleen Bennett
Program Assistant
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Victoria Fonseca
Program Assistant
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Goldie Gorski*
Director of Operations and Outreach
Northwestern-Argonne Institute of Science and Engineering
Northwestern University

Janet Boland*
Executive Assistant
Institute for Molecular Engineering
University of Chicago

Erika Odlaug*
Program Assistant
Northwestern-Argonne Institute of Science and Engineering
Northwestern University



23. CHiMaD-NIST Collaborators

James Warren
Techincal Program Director, Materials Genomics
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Debra Audus
Chemical Engineer, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Chandler Becker
Materials Research Engineer, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Mary Brady
Group Leader, Information Systems Group
Software and Systems Division
Information Technology Laboratory
NIST, Gaithersburg, MD

Benjamin Burton
Research Scientist, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Carelyn Campbell
Group Leader, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Chelsea Davis
NRC Postdoctoral Fellow, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Albert Davydov
Leader, Functional Nanostructured Materials Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Dean DeLongchamp
Researcher, Polymers Processing Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Andrew Dienstfrey
Research Scientist
Mathematical Analysis and Modeling Group
Information Technology Laboratory
NIST, Gaithersburg, MD

Alden Dima
Research Scientist
Software and Systems Division
Information Technology Laboratory
NIST, Gaithersburg, MD

Jack Douglas
NIST Fellow
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Aaron Forster
Materials Research Engineer, Polymeric Materials Group
Materials and Structural Systems Division
Engineering Laboratory
NIST, Gaithersburg, MD

Douglas Fox
Guest Researcher, Flammability Reduction Group
Fire Research Division
Engineering Laboratory
NIST, Gaithersburg, MD

Jeffrey Gilman
Polymer Chemist, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Martin Green
Leader, Materials for Energy and Sustainable Development Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Jonathan Guyer
Group Leader, Mechanical Performance Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Robert Hanisch
Director
Office of Data and Informatics
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Adam Hannon
NRC Postdoctoral Fellow, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Ursula Kattner
Physical Scientist, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Trevor Keller
Postdoctoral Researcher, Mechanical Performance Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Ketan Khare
Postdoctoral Researcher, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Joseph Kline
Project Leader, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Kenneth Kroenlein
Director, Thermodynamic Research Center
Applied Chemicals and Materials Division
NIST, Boulder, CO

Sergiy Krylyuk
Guest Researcher, Functional Nanostructured Materials Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Aaron Gilad Kusne
Researcher, Materials for Energy and Sustainable Development Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Eric Lass
Materials Research Engineer, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Sheng Yen Li
Postdoctoral Researcher Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Lyle Levine
Project Leader, Additive Manufacturing of Metals
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Alexander Liddle
Deputy Director (Acting) and Group Leader
Nanofabrication Research Group
Center for Nanoscale Science and Technology
NIST, Gaithersburg, MD

Li Ma
Guest Scientist, Mechanical Performance Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Kil-Won Moon
Postdoctoral Researcher, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Nhan Van Nguyen
Physicist
Nanoelectronics Group in the Engineering Physics Division
Physical Measurement Laboratory
NIST, Gaithersburg, MD

Sarala Padi
Research Scientist
Software and Systems Division
Information Technology Laboratory
NIST, Gaithersburg, MD

Adele Peskin
Research Scientist
Software and Systems Division
Information Technology Laboratory
NIST, Gaithersburg, MD

Frederick Phelan
Chemical Engineer, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Raymond Plante
Research Scientist
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Vivek Prabhu
Chemical Engineer, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Lee Richter
Physicist, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Deepak Sharma
Guest Researcher, Functional Nanostructured Materials Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Arunima Singh
Guest Researcher, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Christopher Soles
Leader, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Chad Snyder
Research Chemist, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Mark Stoudt
Materials Research Engineer
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Daniel Sunday
Staff Member, Functional Polymers Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Francesca Tavazza
Research Scientist, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Kimberly Tryka
Research Data Librarian, Digital Services and Publishing Group
NIST Research Library
NIST, Gaithersburg, MD

Daniel Wheeler
Researcher, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Maureen Williams
Materials Scientist, Thermodynamics and Kinetics Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Jonathan Winterstein
Research Scientist, Nanofabrication Research Group
Center for Nanoscale Science and Technology
NIST, Gaithersburg, MD

Jeremiah Woodcock
Research Chemist, Polymers and Complex Fluids Group
Materials Science and Engineering Division
Materials Measurement Laboratory
NIST, Gaithersburg, MD

Sharief Youssef
Research Scientist
Software and Systems Division
Information Technology Laboratory
NIST, Gaithersburg, MD

24. Information Dissemination

24.1 Low-Dimensional Nanoelectronic Materials

1. **L. J. Lauhon** *(Invited)*, "Chemical and Functional Imaging of 2D Materials and Mixed Dimensional Heterojunctions", Graphene EU-US Workshop on 2D Materials, Heterostructures and Devices, Manchester, UK (10/11/16)
2. **M. C. Hersam** *(Invited)*, "Solution-processed graphene and related two-dimensional nanomaterial inks", Graphene Canada International Conference, Montreal, Canada (10/20/16).
3. **M. C. Hersam** *(Invited)*, "Chemically functionalized two-dimensional nanoelectronic heterostructures," Raman/AFM-Raman/TERS Workshop, Evanston, Illinois, USA (9/27/16).
4. **M. C. Hersam** *(Invited)*, "Chemically modified two-dimensional nanoelectronic heterostructures," Richard P. Van Duyne Symposium, Minneapolis, Minnesota, USA (9/18/16).
5. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," National Institute for Materials Physics Seminar Series, Bucharest, Romania (9/16/16).
6. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," Institute of Microelectronic Technologies Seminar Series, Bucharest, Romania (9/15/16).
7. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," J. Heyrovsky Institute of Physical Chemistry Seminar Series, Prague, Czech Republic (9/12/16).
8. **L. J. Lauhon** *(Invited)*, "Novel Behaviors in Low-Dimensional Materials and Heterostructures", Walter Schottky Institute Seminar, TU Munich, Garching, Germany (8/31/16)
9. **L. J. Lauhon** *(Invited)*, "Novel Behaviors in Low-Dimensional Materials and Heterostructures", Paul Drude Institute Seminar, Berlin, Germany (8/29/16)
10. **M. C. Hersam** *(Plenary)*, "Mixed dimensional nanoelectronic heterostructures," 8th International Conference on Molecular Electronics, Paris, France (8/25/16).
11. **M. C. Hersam** *(Plenary)*, "Solution-processed graphene and related two-dimensional nanomaterial inks," Graphene Industry Technology Summit Forum, Nanning, China

(8/22/16).

12. **M. C. Hersam** *(Invited)*, "Interfacial engineering of two-dimensional nanoelectronic heterostructures," 25th International Materials Research Congress, Cancun, Mexico (8/15/16).
13. **M. C. Hersam** *(Plenary)*, "Mixed dimensional nanoelectronic heterostructures," 25th International Materials Research Congress, Cancun, Mexico (8/15/16).
14. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," Ajou University BK21 Seminar Series, Suwon, Korea (7/11/16).
15. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," National University of Singapore Centre for Advanced 2D Materials Seminar Series, Singapore, Singapore (7/8/16).
16. **M. C. Hersam** *(Invited)*, "Mixed dimensional nanoelectronic heterostructures," International Conference on Electronic Materials, Singapore, Singapore (7/7/16).
17. **M. C. Hersam** *(Plenary)*, "Mixed dimensional nanoelectronic heterostructures," 58th Electronic Materials Conference, Newark, Delaware, USA (6/22/16).
18. **M. C. Hersam** *(Invited)*, "Mixed dimensional nanoelectronic heterostructures," 229th Electrochemical Society Meeting, San Diego, California, USA (6/1/16).
19. **M. C. Hersam** *(Invited)*, "Chemically modified two-dimensional nanoelectronic heterostructures," 229th Electrochemical Society Meeting, San Diego, California, USA (6/1/16).
20. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," Argonne National Laboratory 2D Materials Beyond Graphene Workshop, Argonne, Illinois, USA (5/11/16).
21. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," Pennsylvania State University Graphene and Beyond Workshop, State College, Pennsylvania, USA (5/10/16).
22. **M. C. Hersam** *(Invited)*, "Van der Waals heterostructures based on two-dimensional and mixed-dimensional nanomaterials," European Materials Research Society Spring Meeting, Lille, France (5/4/16).
23. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," Rice University Materials Science and Nanoengineering Seminar Series, Houston, Texas, USA (4/7/16).
24. **M. C. Hersam** *(Invited)*, "Surface engineering of two-dimensional nanoelectronic heterostructures," 251st American Chemical Society National Meeting, San Diego, California, USA (3/16/16).
25. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of two-dimensional nanoelectronic heterostructures," KAUST-NSF Workshop on Electronic Materials, KAUST, Saudi Arabia (3/14/16).
26. **L. J. Lauhon** *(Invited)*, "Novel Behaviors in Low-Dimensional Materials and Heterostructures", MIE Department Seminar University of Illinois Chicago, Chicago, Illinois, USA (3/1/16)
27. **M. C. Hersam** *(Invited)*, "Processing and properties of low-dimensional nanomaterial heterostructures," Illinois State University Department of Physics Colloquium Series, Normal, Illinois, USA (2/16/16).
28. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," University of Tokyo Institute for Solid State Physics Seminar Series, Tokyo, Japan (2/10/16).

29. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," Gunma University Faculty of Science and Technology Colloquium, Gunma, Japan (2/9/16).
30. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," Michigan Technological University Physics Department Colloquium, Houghton, Michigan (2/4/16).
31. **M. C. Hersam** *(Invited)*, "Fundamentals and applications of low-dimensional nanoelectronic heterostructures," Rochester Institute of Technology Dean"s Distinguished Seminar Series, Rochester, New York, USA (1/28/16).
32. **M. C. Hersam** *(Invited)*, "Mixed dimensional nanoelectronic heterostructures," Argonne National Laboratory Materials Science Division Colloquium Series, Lemont, Illinois, USA (1/14/16).

24.2 Polymer Matrix Materials

1. **W. Chen** *(Invited)* "Design of Engineered Materials Systems", Mechanical Engineering, University of Wisconsin Madison, WI, USA (2/25/16).
2. **H. Wu**, M. Han, E. Luijten, "Dielectric effects on the ion distribution near a Janus colloid", APS March Meeting, Baltimore, MD, USA (03/14/16)
3. **Z. Wang**, E. Luijten, "Dipolar fluids near a dielectric surface", APS March Meeting, Baltimore, MD, USA (03/14/16)
4. **M. Han**, E. Luijten, "Active colloids propelled by induced-charge electrophoresis", APS March Meeting, Baltimore, MD, USA (03/14/16)
5. **Z. Wei**, E. Luijten, "Coarse-grained Simulation of Complexation between Small Interfering RNA and Polycations", APS March Meeting, Baltimore, MD, USA (03/14/16)
6. **R. Zhao** *(Invited)*, L. C. Brinson, L. S. Schadler, X. Li, W. Chen, "NanoMine: A Data Resource for Polymer Nanocomposite Materials", NU-NIMS Materials Genome Workshop, Evanston, IL, USA (3/24/16).
7. **L. C. Brinson**, , R. Zhao, X. Li, W. Chen, "Application of NanoMine Data Resource to Analysis of Interphase Mechanism in Polymer Nanocomposites", Materials Research Society (MRS) Meeting, Phoenix, AZ, USA (3/28/16).
8. **L. C. Brinson**, W. Chen, R. Zhao, "Development of Material Data Resource and Analysis for Polymer Nanocomposites" ICMEg Conference (Integrated Computational Materials Engineering), Barcelona, Spain, (4/13/16).
9. **L. C. Brinson** *(Plenary)*, P. Kolluru, M. Zhang, X. Li, "Local Polymer Properties at Interfaces, Mechanics of Time Dependent Materials Conference", Paris, France, (5/17/16)."
10. **P. V. Kolluru**, M. Zhang, L. C. Brinson, "Measuring the Distribution of Local Interphase Mechanical Properties in Model Nanocomposites", Society for Experimental Mechanics Annual Conference, Orlando, FL, (6/6/16).
11. **L. C. Brinson** *(Invited)*, L. S Schadler, R. Zhao, X. Li, "Stalking the Materials Genome: A Data Driven Approach to the Virtual Design of Nanostructured Polymers", ACS Polymer Composites Conference, Sonoma CA, USA (7/25/16).
12. **E. Luijten**, "Dynamic collective behavior and phase separation of active colloids", University of Science and Technology, Hefei, China (8/18/16)
13. **P. V. Kolluru**, M. D. Eaton, M. Zhang, D. W. Collinson, L. C. Brinson, "Resolving the Distribution of Local Mechanical Properties across Polymer Nanocomposite

Interphases via Novel AFM-based Indentation Experiments", Society for Engineering Science Annual Conference, College Park, MD, (9/2/16).

14. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", MGI seminar series, NIST, Gaithersburgh, MD, USA (9/7/16)
15. **M. Zhang**, S. Askar, J. M. Torkelson, L. C. Brinson, "Explore the Confinement Effect on Local Mechanical Properties of Polymer in Thin Film systems", Society for Engineering Science Annual Conference, College Park, MD, 10/2/16.
16. **W. Chen** *(Distinguished Seminar)* "Design of Engineered Materials Systems", UTC institute for Advanced System Engineering, University of Connecticut, CT, USA (10/17/16).
17. **R. Zhao** *(Invited)*, L. C. Brinson, L. S. Schadler, X. Li, W. Chen, "NanoMine: A Data Resource for Polymer Nanocomposite Materials", Materials Data and Analytics for Materials Research Summit, Evanston, IL, USA (10/31/16).
18. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", Materials Science and Engineering colloquium, University of Illinois at Urbana-Champaign, IL, USA (11/7/16)
19. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", Opening Workshop for Center for Soft Matter, Shanghai Jiao Tong University, Shanghai, China (12/12/16)
20. **S. Keten** *(Invited)* "Understanding Nanoconfinement and Interfaces in Nanocomposites", ASME IMECE Conference, Phoenix, AZ, USA (2016)
21. **S. Keten** *(Invited)* "Understanding Nanoconfinement and Interfaces in Nanocomposites", USACM Workshop on Recent Advances in Computational Methods for Nanoscale Phenomena, Ann Arbor, MI, USA (2016).
22. **S. Keten** *(Invited)*, "Understanding Nanoconfinement and Interfaces in Nanocomposites", 1st International Symposium on Materials from Renewables, Fargo, ND, USA (2016).
23. **S. Keten** *(Invited)*, "Understanding Nanoconfinement and Interfaces in Nanocellulose Composites", Tech Connect World Innovation Conference, Washington, DC, USA (2016).
24. **S. Keten** *(Invited)*, "Understanding Nanoconfinement and Interfaces in Structural Materials", Air Force Research Laboratory, Dayton, OH, USA (2016).
25. **S. Keten** *(Invited)*, "Using polymer conjugation to dictate order and functionality in self-assembling peptides", American Physical Society March Meeting, Baltimore, MD, USA (2016).
26. **S. Keten** *(Invited)*, "Mesoscale Modeling of the Interfacial Mechanics of Nanocellulose Composites - Discerning the role of nanoconfinement", Materials Research Society Fall Meeting, Boston, MA, USA (2015).
27. **S. Keten** *(Invited)*, "Mesoscale Modeling of the Interfacial Mechanics of Nanocellulose Composites - Discerning the role of nanoconfinement", Materials Science Fundamentals Seminar Series, The Dow Chemical Company, Collegeville, PA, USA (2015).
28. **S. Keten** *(Invited)*, "Mesoscale Modeling of the Interfacial Mechanics of Nanocellulose Composites", TAPPI International Conference on Nanotechnology for Renewable Materials, Atlanta, GA, USA (2016).

24.3 Directed Self-assembly of Block Copolymer Films for Lithography

1. **X. Chen**, Seo, T.; Rincon-Delgadillo, P.A.; Matsumiya, T.; Kawaue, A.; Maehashi, T.; Dazai, T.; Gronheid, R.; Nealey, P.F.; "Directed self-assembly of PS-b-PMMA with ionic liquid addition", Advances in Patterning Materials and Processes, SPIE, (2/24/16)
2. **G. S. Khaira**, Doxastakis, M.; Bowen, A.; Ren, J.; Suh, H. S.; Segal-Peretz, T.; Ferrier, N. J.; Vishwanath, V.; Sunday, D. F.; Kline, R. J.; Nealey, P.F.; de Pablo, J.J.. "Molecular simulations and evolutionary computing to reconstruct the block-copolymer morphology from x-ray scattering", Advances in Patterning Materials and Processes, SPIE, (2/25/16)
3. **P. Nealey** *(Invited)*, "Directed Self-Assembly" Institute for Molecular Engineering Day at Argonne National Laboratory, Lemont, IL, USA (2/16)
4. **T. Segal-Peretz**, J. Ren, S. Xiong, G. Khaira, A. Bowen, L. E. Ocola, R. Divan, M. Doxastakis, N. J. Ferrier, J. de Pablo, P. F. Nealey, "Understanding Three Dimensional Assembly in Directed Self-Assembled Block Copolymer films: a Quantitative TEM Tomography Study MRS spring meeting", (3/28/16)
5. **P. Nealey** *(Invited)*, "New block copolymer materials (and processes) for BPM" Advanced Storage Technology Consortium, Santa Clara, CA, USA (3/16)
6. **P. Nealey** *(Invited)*, "Directed Assembly of Performance Materials" American Physical Society March Meeting, Baltimore, MD, USA (3/16)
7. **H. Jaeger** *(Invited)*, "Granular Dynamics: From Fundamental Science to Practical Applications, short course for industry", Houston, TX, USA (4/13/16)
8. **M. Doxastakis**, Khaira, G. S.; Bowen, A.; Ren, J.; Suh, H. S.; Segal-Peretz, T.; Sunday, D. F.; Kline, R. J.; Nealey, P.F.; de Pablo, J.J.. "Simulations at the interface: association, adsorption, reaction and diffusion", University of Tennessee Knoxville and Virginia Tech Polymer Workshop, (4/18/16)
9. **P. Nealey** *(Invited)*, "Future Science: Small Scale, Big Impact" UChicago Discovery Series, Chicago, IL , USA (4/16)
10. **P. Nealey** *(Invited)*, "Directed Assembly of Performance Materials" Department of Materials Science, Cornell University, Ithaca, NY, USA (4/16)
11. **P. Nealey** *(Invited)*, "Structure-function relationship of block copolymer electrolytes: anisotropy and interconnectivity", Materials Division Energy Day, Argonne National Laboratory, Lemont, IL, USA (4/16)
12. **H. Jaeger** *(Invited)*, "Jamming by Design", Burstein Lecture (colloquium), University of Pennsylvania, PA, USA (5/6/16)
13. **T. Segal-Peretz**, J. Ren, C. Zhou, S. Xiong, G. Khaira, A. Bowen, L. E. Ocola, R. Divan, M. Doxastakis, N. J. Ferrier, J. de Pablo, P. F. Nealey, "Underneath the surface of block copolymer thin films" APS/CNM user meeting, Lemont, IL, USA(5/9/16)
14. **P. Nealey** *(Invited)*, "Enjoy the process", Symposium in honor of Robert E. Cohen, MIT, MA, USA (5/16)
15. **P. Nealey** *(Invited)*, "Interface-defined matter, Basic Research Needs Workshop on Synthesis Science for Energy Relevant Technology", Washington DC, USA (5/16)
16. **P. Nealey** *(Invited)*, "Directed self-assembly (DSA) of performance materials", EUPOC 2016, Block Copolymers for Nanotechnology Applications, Gargnano, Italy, (6/16)
17. **P. Nealey** *(Invited)*, "Self-aligned DSA of multi-color manufacturing-relevant patterns", Tokyo Ohka Kogyo Co., Ltd., Kanagawa-ken, Japan (6/16)

18. **T. Segal-Peretz**, J. Ren, S. Xiong, G. Khaira, A. Bowen, L. E. Ocola, R. Divan, M. Doxastakis, N. J. Ferrier, J. de Pablo, P. F. Nealey, "Underneath the surface of block copolymer thin films: understanding three dimensional assembly in directed self-assembled films using electron tomography", GRC polymer physics, (6/24/16)
19. **H. Jaeger** *(Invited)*, "Granular Materials by Design: Mapping desired properties of the aggregate to properties of individual particles, conference presentation", Granular Matter: Gordon Research Conference, Easton, MA, USA (7/24/16)
20. **P. Nealey** *(Invited)*, "Directed Self-Assembly of Block Copolymer Thin Films", Polymer Physics Gordon Conference, South Hadley, MA, USA (7/16)
21. **P. Nealey** *(Invited)*, "Three dimensional structure in directed self-assembly of block copolymers", International Conference of Photopolymer Science and Technology, Chiba, Japan (7/16)
22. **P. Nealey** *(Invited)*, "Solvent-Assisted Non-Equilibrium Directed Self-Assembly of Complex Polymeric Materials", Department of Energy Materials Chemistry PI's Meeting, Gaithersburg, MD, USA (7/16)
23. **H. Jaeger** *(Invited)*, "Visualizing velocity in jamming fluids, workshop presentation", NIST-CHiMaD Workshop on Impact Mitigating Materials for Body Protection, Chicago, IL, USA (8/8/16)
24. **J. Raybin**, S, Sibener, "Real-Time AFM of Block Copolymer Self Assembly", American Vacuum Society - Prairie Chapter, Illinois Institute of Technology, Chicago, IL, USA (9/8/16)
25. **P. Nealey** *(Invited)*, "Directed Self-Assembly of Performance Materials", Polymer Science and Engineering, University of Massachusetts, Amherst, MA, USA (9/16)
26. **P. Nealey** *(Invited)*, "Directed Self-Assembly of Performance Materials", KAIST, Daejon, Korea (10/16)
27. **P. Nealey** *(Invited)*, "Directed Self-Assembly of Performance Materials", Polymer Society of Korea 40th Anniversary, Jeju Island, Korea (10/16)
28. **P. Nealey** *(Invited)*, "Metrology-based design of materials and processes for DSA", DSA Workshop, Grenoble, France (10/16)
29. **P. Nealey** *(Invited)*, "Directed Self-Assembly of Performance Materials", Institute Lecture, Grenoble Nanoscience Foundation, Grenoble, France (10/16)
30. **H. Jaeger** *(Invited)*, "Granular Materials by Design: Mapping desired properties of the aggregate to properties of individual particles", IIT Mechanical, Materials and Aerospace Engineering Department Seminar, Chicago, IL, USA (11/2/16)
31. **H. Jaeger** *(Keynote)*, "Dynamic solidification of dense suspensions under shear", AIChE Meeting, San Francisco, CA, USA (11/14/16)
32. **S. Sibener** *(Invited)*, Department of Chemistry and Biochemistry Seminar, Montana State University, Bozeman, MT, USA
33. **S. Sibener** *(Invited)*, Department of Chemical Engineering Seminar, University of Illinois - Chicago, Chicago, IL, USA
34. **S. Sibener** *(Invited)*, Department of Chemistry/Chemical Biology Seminar, University of New Mexico, Albuquerque, NM, USA
35. **S. Sibener** *(Invited)*, Scattering of Atoms and Molecules from Surfaces (SAMS-3), Bergen, Norway
36. **S. Sibener** *(Invited)*, Department of Chemistry and Biochemistry Seminar, Andrews University, Berrien Springs, MI, USA

24.4 Additive Manufacturing Seed Group

1. **J. Cao**, "Mechanical Testing and Properties", Measurement Science for Additive Manufacturing, NIST Workshop on Measurement Science for Directed Energy Deposition, Evanston, IL, USA (5/23/16)
2. **J. Bennett**, R. Dudas, J. Cao, K. Ehmann, G. Hyatt, "Control of Heating and Cooling for Direct Laser Deposition Repair of Cast Iron Components", International Symposium on Flexible Automation, Cleveland, OH, USA (8/1/16)

24.5 Soft Matter Design Based on Charge Complexation

1. **M.V. Tirrell**, "Polyelectrolyte Complexation: New Physics and New Materials", Edward J. Kramer Memorial Symposium, Santa Barbara, CA, USA (1/16)
2. **S. Srivastava**, M. V. Tirrell, "Self-Assembly in Polyelectrolyte Complex Hydrogels", Annual Meeting of the American Physical Society, Baltimore, MD, USA (3/16)
3. **H-K. Kwon** *(Poster)*, B. Ma, V. Pryamitsyn, and M. Olvera de la Cruz, "Multiscale modeling of ionic copolymers and blends," CHiMaD Annual Meeting, CHiMaD Headquarters, Evanston, IL, USA (3/23/16)
4. **H-K. Kwon**, J. W. Zwanikken, K. R. Shull, M. Olvera de la Cruz, "The effect of ionic correlations on the distribution of ions across the polyelectrolyte blend interface," Oral Presentation, American Physical Society March Meeting, Baltimore, MD, USA (3/16)
5. **M. Olvera de la Cruz** *invited*, J. Zwanikken and H. Kwon, "Multiple phase co-existence in polymer electrolytes" ACS National Meeting, San Diego, CA, USA (3/13/16)
6. **S. Srivastava**, J. J. de Pablo, M. V. Tirrell et al, "Complexation Driven Block Copolyelectrolyte Self-Assembly", ACS Colloid & Surf. Sci. Symposium, Boston, MA, USA (6/16)
7. **H-K. Kwon** *(Poster)*, J. W. Zwanikken, K. R. Shull, M. Olvera de la Cruz, "Ionic correlation-induced phase behavior in binary and ternary blends of polyelectrolytes", Polymer Physics - Gordon Research Conference, Mt. Holyoke, MA, USA (7/16)
8. **S. Srivastava** *(Poster)*, M. Andreev, A. Levi, J. J. de Pablo and M. V. Tirrell, "Polyelectrolyte Complexation Driven Self-Assemblies: Micelles, Networks and Hydrogels", Polymer Physics-Gordon Research Conference, South Hadley, (7/16)
9. **M.V. Tirrell** *(Invited)*, "Polyelectrolyte Complexation: New Physics and New Materials", American Chemical Society Meeting, Philadelphia, PA, USA (8/16)
10. **M.V. Tirrell** *(Invited)*, "Polyelectrolyte Complexation: New Physics and New Materials", Peking University, Peking, China (9/16)
11. **H-K. Kwon**, J. W. Zwanikken, K. R.Shull, M. Olvera de la Cruz "Solubility of Salt in Polyelectrolyte Blends Soft Matter Design based on Charge Complexation" Mini Symposium, Institute for Molecular Engineering, The University of Chicago, Chicago, IL, USA (10/21/16).
12. **S. Srivastava**, M. Andreev, A. Levi, J. J. de Pablo and M. V. Tirrell, "Polyelectrolyte Complexation Driven Self-Assembly", Annual Meeting of the Annual Meeting of AIChE, San Francisco, CA, USA (11/16)
13. **S. Srivastava** *(Poster)*, M. Andreev, A. Levi, J. J. de Pablo and M. V. Tirrell, "Polyelectrolyte Complexation Driven Self-Assemblies: Micelles, Networks and Hydrogels" Annual Meeting of the Annual Meeting of AIChE, San Francisco, CA, USA (11/16)

14. **H. Wu**, M. Han, E. Luijten, "Dielectric effects on the ion distribution near a Janus colloid", APS March Meeting, Baltimore, MD, USA (03/14/16)
15. **Z. Wang**, E. Luijten, "Dipolar fluids near a dielectric surface", APS March Meeting, Baltimore, MD, USA (03/14/16)
16. **M. Han**, E. Luijten, "Active colloids propelled by induced-charge electrophoresis", APS March Meeting, Baltimore, MD, USA (03/14/16)
17. **Z. Wei**, E. Luijten, "Coarse-grained Simulation of Complexation between Small Interfering RNA and Polycations", APS March Meeting, Baltimore, MD, USA (03/14/16)
18. **E. Luijten**, "Dynamic collective behavior and phase separation of active colloids", University of Science and Technology, Hefei, China (8/18/16)
19. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", MGI seminar series, NIST, Gaithersburgh, MD, USA (9/7/16)
20. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", Materials Science and Engineering colloquium, University of Illinois at Urbana-Champaign, IL, USA (11/7/16)
21. **E. Luijten**, "From self-assembly to electrokinetics: Novel predictive capabilities for dielectric effects", Opening Workshop for Center for Soft Matter, Shanghai Jiao Tong University, Shanghai, China (12/12/16)

24.6 NIST-CHiMaD Postdoctoral Research Fellows

1. **M. Andreev** (*Poster*),"Coarse-grained model for phase behavior of polyelectrolyte solutions", MGI program review (2/5/16)
2. **M. Andreev**,"Coarse-grained molecular dynamics of a charged polymer coacervates", CHiMaD Biomaterials meeting,(3/11/16)
3. **M. Andreev** (*Poster*),"Coarse-grained molecular dynamics of a charged polymer coacervate", CHiMaD annual meeting (3/23/16)
4. **M. Andreev**, "Charged copolymers complexation", CHiMaD meeting, (7/10/16)
5. **M. Andreev**,"Charged copolymers complexation", Prabhu Group Meeting, NIST, Gaithersburgh, MD, USA (8/11/16)
6. **M. Andreev**,"Modeling added salt influence on polyelectrolyte dynamics" NIST COMSOFT meeting, Gaithersburgh, MD, USA (8/31/16)
7. **M. Andreev**,"Coarse-grain molecular dynamics study of charged polymers", CHiMaD mini-symposium, (10/10/16)
8. **N. Ofori-Opoku**, "Phase-field crystal modeling", CEA, Saclay, France (5/16)
9. **N. Ofori-Opoku**, "Phase-field crystal modeling - a continuum atomistic formalism on diffusive time scales", Ecole Centrale Paris, Chatenay-Malabry, France (5/16)
10. **N. Ofori-Opoku**, "Multi-scale Modeling of Precipitation Reactions Using Phase-field Crystal", MS&T Technical Meeting & Exhibition, Salt Lake City, Utah, USA (10/16)
11. **N. Ofori-Opoku**, "A Description of Faceting Surfaces and Multi-Scale Modeling of Precipitation Using Phase- Field Crystal", Department Materials Science and Engineering, University of Virginia, Charlottesville, Virginia, USA (11/16)
12. **W. Xia**, "Predicting thermomechanical response of polymer thin films and nanocomposites via an innovative coarse-grained approach", APS March Meeting, Baltimore, MD, USA (3/15/16)
13. **W. Xia**, "Designing multi-layer graphene-based assemblies for enhanced toughness

in nacre-inspired nanocomposites", SES Technical Meeting, College Park, MD, USA (10/03/16)

24.7 Materials Data Facility

1. **B. Blaiszik**, I. Foster, K. Chard "Demonstration of Globus Research Data Management Services and The Materials Data Facility", Advanced Photon Source Data Seminar, Argonne National Laboratory, Lemont, IL, USA (1/16)
2. **M. Ondrejcek**, B. Blaiszik, K. Chard, J. Pruyne, R. Ananthakrishnan, J. Towns, K. McHenry, S. Tuecke, I. Foster. "Materials Data Facility - Data Services to Advance Materials Science Research", T2C2 DIBBS Meeting, University of Illinois at Urbana-Champaign, Urbana, IL, USA (2/16)
3. **B. Blaiszik** (*Invited*), K. Chard, J. Pruyne, R. Ananthakrishnan, J. Towns, S. Tuecke, I. Foster. "Materials Data Facility - Data Services to Advance Materials Science Research", TMS 2016, Nashville, TN, USA (2/16)
4. **B. Blaiszik** (*Keynote*), K. Chard, J. Pruyne, R. Ananthakrishnan, J. Towns, S. Tuecke, I. Foster. "Materials Data Facility - Data Services to Advance Materials Science Research", DOE National Multimodal Data Analysis Workshop, Lemont, IL, USA (02/16)
5. **B. Blaiszik**, K. Chard, J. Pruyne, R. Ananthakrishnan, K. McHenry, M. Ondrejcek, J. Towns, S. Tuecke, I. Foster. "Materials Data Facility Hands-on Training Workshop", NIST/CHiMaD Data Workshop, Evanston, IL, USA (5/16)
6. **B. Blaiszik** (*Invited*), K. Chard, J. Pruyne, R. Ananthakrishnan, K. McHenry, M. Ondrejcek, J. Towns, S. Tuecke, I. Foster. "Materials Data Facility - Data Services to Advance Materials Science Research", Advanced Photon Source National Users Meeting, Lemont, IL, USA (5/16)
7. **B. Blaiszik** (*Invited*), K. Chard, J. Pruyne, R. Ananthakrishnan, K. McHenry, M. Ondrejcek, J. Towns, S. Tuecke, I. Foster. "Materials Data Facility - Data Services to Advance Materials Science Research", CyberFab National Workshop, Champaign, IL, USA (5/16)
8. **I. Foster**, B. Blaiszik, "Integrating the Materials Data Facility with DOE's ElectroCat Project", ElectroCat Workshop, Lemont, IL, USA (6/16)
9. **S. Tuecke**, V. Vasiliadis, R. Ananthakrishnan "GlobusWorld Tour - San Francisco Bay Area", Lawrence Berkeley National Lab, Berkeley, CA, USA (9/16)
10. **B. Blaiszik**, I. Foster "The Materials Data Facility". TMS National Webinar Series on Materials Data Curation Tools (9/16)
11. **B. Blaiszik** "Globus, Big Data Publication, and the Materials Data Facility", Hands-on training session at the Midwest Big Data Hub Meeting, Rosemont, IL, USA (10/16)
12. **S. Tuecke**, V. Vasiliadis, "Globus 101 Webinar". YouTube Webinar (>750 views) includes data publication demo, online. [https://www.youtube.com/watch?v=K17ZZEIvWhg] (10/16)
13. **S. Tuecke**, V. Vasiliadis, R. Ananthakrishnan "GlobusWorld Tour - New York/Connecticut Area", Yale Center for Research Computing, New Haven, CT, USA. (10/16)
14. **S. Tuecke**, V. Vasiliadis, R. Ananthakrishnan "GlobusWorld Tour - Colorado Area", National Center for Atmospheric Research, Boulder, CO, USA (10/16)

24.8 Impact Mitigation

1. **H. Jaeger** *(Invited)*, "Granular Dynamics: From Fundamental Science to Practical Applications, short course for industry", Houston, TX, USA (4/13/16)
2. **H. Jaeger** *(Invited)*, "Jamming by Design", Burstein Lecture (colloquium), University of Pennsylvania, PA, USA (5/6/16)
3. **H. Jaeger** *(Invited)*, "Granular Materials by Design: Mapping desired properties of the aggregate to properties of individual particles, conference presentation", Granular Matter: Gordon Research Conference, Easton, MA, USA (7/24/16)
4. **H. Jaeger** *(Invited)*, "Visualizing velocity in jamming fluids, workshop presentation", NIST-CHiMaD Workshop on Impact Mitigating Materials for Body Protection, Chicago, IL, USA (8/8/16)
5. **S. Nagel** *(Invited)*, "Directing force/energy through architecture", NIST-CHiMaD Workshop on Impact Mitigating Materials for Body Protection, Chicago, IL, USA (8/8/16)
6. **H. Jaeger** *(Invited)*, "Granular Materials by Design: Mapping desired properties of the aggregate to properties of individual particles", IIT Mechanical, Materials and Aerospace Engineering Department Seminar, Chicago, IL, USA (11/2/16)
7. **H. Jaeger** *(Keynote)*, "Dynamic solidification of dense suspensions under shear", AIChE Meeting, San Francisco, CA, USA (11/14/16)

24.9 Phase Field Methods

1. **M. J Welland**, D.T. O'Connor, D. Karpeyev, P. W. Voorhees, O. Heinonen, "Miscipbility gap closure, interface morphology, and phase microstructure of Li_xFePO_4 from surface wetting and strain", American Ceramics Society Electronic Materials and Applications, Orlando, FL, USA (1/20/16)
2. **S. O. Poulsen**, P. W. Voorhees, "A Verified Phase Field Method for Phase Transformations in Ni-Cr-Al Alloys, Plasticity", International Conference on Plasticity, Damage and Fracture 2016, Keauhou Bay, Hawaii (1/16)
3. **K. McReynolds**, P. W. Voorhees, G.B. Olson and J. dePablo, "From The Center for Hierarchical Materials Design to a New Tool for Materials Simulation", National Institute for Materials Science, Japan (3/16)
4. **N. Ofori-Opoku**, "Phase-field crystal modeling", CEA, Saclay, France (5/16)
5. **N. Ofori-Opoku**, "Phase-field crystal modeling - a continuum atomistic formalism on diffusive time scales", Ecole Centrale Paris, Chatenay-Malabry, France (5/16)
6. **M. C. Peters**, J. W. Doak, J. E. Saal, G. B. Olson, P. W. Voorhees, "Thermodynamic modeling of PbX (X=S,Te) using a five sub-lattice model developed explicitly for semiconductors", CALPHAD Meeting, Japan, (6/16)
7. **N. Ofori-Opoku**, "Multi-scale Modeling of Precipitation Reactions Using Phase-field Crystal", MS&T Technical Meeting & Exhibition, Salt Lake City, Utah, USA (10/16)
8. **N. Ofori-Opoku**, "A Description of Faceting Surfaces and Multi-Scale Modeling of Precipitation Using Phase- Field Crystal", Department Materials Science and Engineering, University of Virginia, Charlottesville, Virginia, USA (11/16)

24.10 Presentations on Center for Hierarchical Materials Design

1. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. de Pablo, The Center for Hierarchical

Materials Design: Realizing the Promise of the Materials Genome Initiative, SIP-Structural Materials for Innovation Review, Japan Science and Technology Office, Japan (2/16)

2. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. de Pablo, The Center for Hierarchical Materials Design: Realizing the Promise of the Materials Genome Initiative, Opening Ceremony Research Center for the Computational Design of Advanced Functional Materials, National Institute for Advanced Industrial Science and Technology, Japan (2/16)
3. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. de Pablo, The Center for Hierarchical Materials Design: Realizing the Promise of the Materials Genome Initiative, National Academy of Engineering-American Association of Engineering Societies, Washington DC, USA (4/16)
4. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. de Pablo, The Center for Hierarchical Materials Design: Realizing the Promise of the Materials Genome Initiative, Institute for Materials Research, Materials Week Ohio State University, OH, USA (5/1)
5. **E. B. Gulsoy**, P. W. Voorhees, G.B. Olson and J. de Pablo, The Center for Hierarchical Materials Design: An Overview, CHiMaD MGI Toolkit and Materials Design Training, Carnegie Mellon University, Pittsburgh, PA, USA (6/8)
6. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. de Pablo, The Center for Hierarchical Materials Design: Realizing the Promise of the Materials Genome Initiative, CINEMA meeting, Copenhagen, Denmark (9/15)
7. **P.W. Voorhees** *(Invited)*, G.B. Olson and J. dePablo, The Center for Hierarchical Materials Design: Realizing the Promise of the Materials Genome Initiative, National Institute for Materials Science, NIMS Week, Japan (10/25)

24.11 Organic Bulk Heterojunction Polymer Solar Cells

1. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, Texas A&M University Qatar Campus, Qatar (1/16)
2. **M. Goldey**, G. Galli, Electronic structure properties as signatures of morphological motifs in organic photovoltaics. American Physical Society March Meeting, Baltimore, MD, USA. (3/16/16)
3. **M. Goldey** *(Poster)*, D. Reid, J. de Pablo, G. Galli, Organic photovoltaic modeling, Center for Hierarchical Materials Design Annual meeting, Evanston, IL, USA (3/23/16)
4. **L. Yu** *(Invited)*, Dipolar Change That Matters-Design ideas for new low band gap polymers for highly efficient solar cells, Eaton Symposium, Unversity of Chicago, Chicago, IL, USA (4/18/16)
5. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, American Chemical Society Spring Meeting, San Diego, CA, USA (4/16)
6. **M. Goldey** *(Poster)*, D. Reid, J. de Pablo, G. Galli, Don't twist that polymer! Organic solar cell structure-property relationships, Car Parrinello Molecular Dynamics 2016, Chicago, IL, USA (5/16/16)
7. **L. Yu** *(Invited)*, The Materials for Solar Technologies symposium, The TechConnect World Innovation Conference, Washington DC, USA (5/22/16)
8. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, University of the Chinese Academy of Sciences, China (5/16)
9. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, American

University of Beirut, Beirut, Lebanon (5/16)

10. **L. Yu** *(Invited)*, Mechanistic Studies of ternary OPV solar cells , Gordon Conference, Hong Kong (6/19/16)
11. **L. Yu** *(Invited)*, Mechanistic Studies of ternary OPV solar cells, 252nd ACS National Meeting & Exposition, Philadelphia, PA, USA (8/21/16)
12. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, American Chemical Society Fall Meeting, Philadelphia, PA, USA (8/16)
13. **L. Yu** *(Invited)*, Progress and Challenges in Polymer OPV Solar Cells, Albuquerque, NM, (9/9/2016)
14. **M. Goldey** *(Poster)*, N. Brawand, M. Voeroes, G.Galli. Shallow and deep traps in Quantum Dot Solids, Argonne Postdoctoral Research and Career Symposium, Lemont, IL, USA (10/6/16)
15. **T. J. Marks** *(Invited)*, Interface Science of Organic Photovoltaic Materials, BK21 International Workshop on Photovoltaics, Korea University, Sejong Campus, Korea (10/16)

24.12 Data Mining

1. **A. Choudhary** *(Invited)*, "Accelerating Discoveries with Big Data and Supercomputing", University of Chicago, Chicago, IL, USA (02/16)
2. **C. Wolverton** *(Invited)*, "High-throughput Computational Search for Strengthening Precipitates in Alloys", TMS Annual Meeting, (2/16)
3. **C. Wolverton** *(Invited)*, "Assessing the Accuracy of DFT Formation Energies", TMS Annual Meeting, (2/16)
4. **A. Agrawal** *(Invited)*, Alok Choudhary, "Towards Better Efficiency and Accuracy: Data Mining for Prediction and Optimization in Materials System Design", TMS 2016, Nashville TN, USA (2/16/16)
5. **L. Ward**, C. Wolverton. "Materials Design with Quantum Mechanics and Machine Learning" University of South Carolina. Guest Lecture for Materials Synthesis and Processing Course (2/11/16)
6. **L. Ward**, C. Wolverton. "Magpie: A Materials-Agnostic Platform for Informatics and Exploration" ICME Infrastructure Development for Accelerated Materials Design: Data Repositories, Informatics, and Computational Tools, TMS 2016, Nashville, TX, USA (2/16/16)
7. **L. Ward**, R. Liu, A. Krishna, V. Hegde, A. Agrawal, A. Choudhary, C. Wolverton. "A General-Purpose Toolkit for Predicting the Properties of Materials using Machine Learning" Computational Materials Discovery and Optimization: From 2D to Bulk Materials, TMS 2016, Nashville, TX, USA (2/17/16)
8. **W. Chen** *Invited*, "Design of Engineered Materials Systems", Mechanical Engineering, University of Wisconsin Madison, Madison, WI, USA (2/25/16)
9. **C. Wolverton** *(Invited)*, American Chemical Society, Philadelphia, PA, USA (3/16)
10. **C. Wolverton** *(Invited)*, German Physical Society, (3/16)
11. **L. Ward**, R. Liu, A. Krishna, V. Hegde, A. Agrawal, A. Choudhary, C. Wolverton. "Accurate Models of Formation Enthalpy Created using Machine Learning and Voronoi Tessellations" Accurate Models of Formation Enthalpy Created using Machine Learning and Voronoi Tessellations, American Physical Society March Meeting 2016, (3/15/16)
12. **A. Agrawal** *(Invited)*, "CHiMaD Data Mining: Fatigue", SRG 2016, Evanston IL,

USA (3/21/16)

13. **A. Agrawal** *(Invited)*, Alok Choudhary, "CHiMaD Data Mining", CHiMaD Annual Meeting, Evanston IL, USA (3/23/16)
14. **A. Paul** *Poster*, A. Furmanchuk, A. Agrawal, A. Choudhary, "Designing optimal OPV devices by modeling Processing-Structure-Property Linkages using Machine Learning" CHiMaD Annual Meeting, Evanston IL, USA (3/23/16)
15. **A. Furmanchuk** *Poster*, A. Agrawal, J. Saal, J. Doak, G. Olson, and A. Choudhary, "Data Mining Tools for Thermoelectric Materials", CHiMaD Annual Meeting, Evanston IL, USA (3/23/16)
16. **A. Krishna**, A. Agrawal, S. Padi, A. Peskin, A. Dima, K. Kroenlein, A. Choudhary, "Classification of Scientific Journal Articles for NIST Thermodynamic Research Center", CHiMaD Annual Meeting, Evanston IL, USA (3/23/16)
17. **C. Wolverton** *(Invited)* Department Colloquium, Washington Univ. at St. Louis, (4/16)
18. **C. Wolverton** *(Invited)*, "Accelerating Materials Discovery with Data-Driven Computational Tools" NIST MGI Seminar Series, NIST, Gaithersburgh, MD, USA (5/16)
19. **C. Wolverton** *(Invited)*, Department Colloquium, Univ. of Washington, Seattle, USA (5/16)
20. **C. Wolverton** *(Invited)*, Department Colloquium, MIT, (5/16)
21. **C. Wolverton** *(Invited)*, Department Colloquium, Johns Hopkins Univ., (5/16)
22. **A. Agrawal** *(Invited)*, "Data-driven materials science enabling large-scale property prediction and optimization", APS/CNM Users Meeting 2016, Argonne National Lab, Chicago IL, USA (5/10/16)
23. **C. Wolverton** *(Invited)*, IU-MRS Meeting, Singapore, (6/16)
24. **C. Wolverton** *(Invited)*, Next Generation Electrochemistry Summer School, UIC (6/16)
25. **C. Wolverton** *(Invited)*, Electrochemical Society Annual Meeting, (6/16)
26. **L. Ward**, S. O'Keeffe, J. Stevick, G. Jelbert, M. Aykol, A. Agrawal, A. Choudhary, C. Wolverton. "Using Machine Learning to Design New Bulk Metallic Glass Alloys," BMG XI, (6/7/16)
27. **A. Agrawal**, Alok Choudhary, "Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science", Theory and Applications of Computational Chemistry (TACC), University of Washington, Seattle WA, USA (8/30/16)
28. **R. Liu**, L. Ward, C. Wolverton, A. Agrawal, W.-K. Liao, and A. Choudhary, "Deep Learning for Chemical Compound Stability Prediction," ACM SIGKDD Workshop on Large-scale Deep Learning for Data Mining (DL-KDD) San Francisco, CA, USA (8/16)
29. **C. Wolverton** *(Invited)*, CAMD Summer School, Copenhagen, Sweden (8/16)
30. **C. Wolverton** *(Invited)*, American Chemical Society Fall Meeting, Philadelphia, PA, USA (8/16)
31. **C. Wolverton** *(Invited)*, IPAM Workshop, "Machine Learning meets Many Particle Problems", UCLA, CA, USA (8/16)
32. **C. Wolverton** *(Invited)*, Vienna Young Researchers Workshop, Vienna, Austria (9/16)
33. **A. Agrawal**, Alok Choudhary "Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science", International Conference on Fatigue Damage of Structural Materials (FATD), Hyannis MA, USA (9/22/16)

34. **C. Wolverton** *(Invited)*, Lorentz Center Workshop, "Open Databases Integration for Materials Design", Leiden, Netherlands (10/16)
35. **W. Chen** *Invited*, "Design of Engineered Materials Systems", UTC institute for Advanced System Engineering, University of Connecticut, Storrs, CT, USA(10/17/16)
36. **A. Agrawal**, Alok Choudhary, "A Fatigue Strength Predictor for Steels Using Ensemble Data Mining", 25th ACM International Conference on Information and Knowledge Management (CIKM), Indianapolis IN, USA (10/26/16)
37. **A. Agrawal** *(Invited)*, "Materials Informatics and Big Data: Realization of the 'Fourth Paradigm' of Science in Materials Science", CHiMaD Summit on Data and Analytics for Materials Research, Evanston IL, USA (11/2/16)
38. **A. Paul** *(Poster)*, A. Furmanchuk, A. Agrawal, A. Choudhary, "Designing optimal OPV devices by modeling Processing-Structure-Property Linkages using Machine Learning" CHiMaD Summit on Data and Analytics for Materials Research, Evanston IL, USA (11/1/16)
39. **A. Furmanchuk**, A. Agrawal, J. Saal, J. Doak, G. Olson, and A. Choudhary, "Machine Learning for Advancing Discovery of Novel Thermoelectric Materials: ThermoEl". AIChE Annual Meeting, San Francisco, CA, USA (11/13/16)
40. **A. Agrawal** B. Meredig, C. Wolverton, and A. Choudhary, "A Formation Energy Predictor for Crystalline Materials Using Ensemble Data Mining," IEEE International Conference on Data Mining (ICDM), Barcelona, Spain (12/13/16)

24.13 Precipitation-Strengthened Alloys

1. **G. B. Olson** *(Invited)*, "Materials Genomics," CHiMaD National Materials Data Workshop, Evanston, IL, USA (1/25/16)
2. **G. B. Olson** *(Invited)*, "Genomic Materials Design: From CALPHAD to Flight" ALCOA Tech Center, Pittsburgh, PA, USA (2/12/16)
3. **G. B. Olson** *(Invited)*, "Genomic Data Infrastructure for Computational Materials Design," TMS Annual Meeting, Nashville TN, USA (2/15/16)
4. **G. B. Olson** *(Invited)*, "Mapping the Thermoelectrics Genome," CHiMaD Thermoelectrics Workshop, Northwestern University, Evanston, IL, USA (2/29/16)
5. **G. B. Olson** *(Invited)*, "Materials Genomics," Honeywell National Security Campus, Kansas City, MO, USA (3/3/16)
6. **G. B. Olson** *(Invited)*, "Precipitation-Strengthened Alloys by Design," CHiMaD Materials Design Center 2nd Annual Review Meeting, Evanston, IL, USA (3/23/16)
7. **G. B. Olson** *(Invited)*, "Metallurgical Design of Concrete and Polymers," 4th NU-NIMS Materials Genome Workshop, Northwestern University, Evanston, IL, USA (3/24/16)
8. **G. B. Olson** *(Invited)*, "Data-Driven Discovery for Designed Thermoelectric Materials," DARPA-SIMPLEX PI Review Meeting, Arlington, VA, USA (4/4/16)
9. **G. B. Olson** *(Invited)*, "Computational Materials Design," Council on Competitiveness, Washington DC, USA (4/12/16)
10. **G. B. Olson** *(Invited)*, "ICME for Corrosion Fatigue," NNL Corrosion Fatigue Modeling Program Review, Albany, NY, USA (4/19/16)
11. **G. B. Olson** *(Invited)*, "Advances in Computational Materials Design," Hero-m Materials Design Center Annual Review, KTH-Stockholm, Sweden (5/10/16)
12. **G. B. Olson** *(Invited)*, "Microstructures, Alloy Design, and SME Transfer," NIST-MSAM Project Closeout Workshop, Northwestern University, Evanston, IL, USA

(5/23/16)

13. **G. B. Olson** *(Invited)*, "Materials Genome Initiative," ASM Materials Education Foundation Meeting, Chicago, IL, USA (6/3/16)
14. **G. B. Olson** *(Invited)*, "Materials Design: From Genome to Flight," NIST-CHiMaD Materials Design Workshop, NIST, Gaithersburg MD, USA (6/13/16)
15. **G. B. Olson** *(Invited)*, "Genomic Materials Design," NIST Management CHiMaD Briefing, Northwestern University, Evasnton, IL, USA (6/28/16)
16. **G. B. Olson** *(Invited)*, "Integrated Computational Materials Design: From Genome to Flight," IUMRS International Conference on Electronic Materials, Singapore (7/5/16)
17. **G. B. Olson** *(Invited)*, "Success Stories in Genomic Materials Design," University/Industry Panel Presentation, Whitehouse MGI Five Year Review, Washington, DC, USA (8/2/16)
18. **G. B. Olson** *(Invited)*, "ICME for Additive Manufacturing," DARPA Open Manufacturing Program Review, Arlington, VA, USA (8/11/16)
19. **G. B. Olson** *(Invited)*, "Data-Driven Discovery for Designed Thermoelectrics," DARPA-SIMPLEX Program Review, Arlington, VA, USA (9/20/16)
20. **G. B. Olson** *(Invited)*, "MGI: Accelerating Materials Technology Transition," Honeywell National Security Campus, Kansas City, MO, USA (9/29/16)
21. **G. B. Olson** *(Invited)*, "DFT Prediction of GB Embrittlement: Application to Al Alloys," Constellium Scientific Advisory Board Meeting, Neuf Brisach, France (10/14/16)
22. **G. B. Olson** *(Invited)*, "AIM Qualification of Additively Manufactured Components," AIM Symposium, MS&T2016, Salt Lake City, Utah, USA (10/24/16)
23. **G. B. Olson** *(Invited)*, "ICME Education at Northwestern," Judd Education Symposium, MS&T2016, Salt Lake City, Utah, (10/24/16)
24. **G. B. Olson** *(Invited)*, "Harnessing the Gibbs Genome: From CALPHAD to Flight," Gibbs Award Symposium, MS&T2016, Salt Lake City, Utah, USA (10/25/16)
25. **G. B. Olson** *(Invited)*, "NeoAlchemy: Transmuting Data into New Materials," Keynote Lecture, CHiMaD International Materials Data Summit, Northwestern University, Evanston, IL, USA (10/31/16)
26. **G. B. Olson** *(Invited)*, "Materials Genomics: Accelerating Materials Innovation," Materials Innovation Panel Presentation, OECD Smart Industry Technology Policy Conference, Stockholm, Sweden (11/17/16)
27. **C. Wolverton** *(Invited)* Department Colloquium, Washington Univ. at St. Louis, (4/16)
28. **C. Wolverton** *(Invited)*, "Accelerating Materials Discovery with Data-Driven Computational Tools" NIST MGI Seminar Series, NIST, Gaithersburgh, MD, USA (5/16)
29. **C. Wolverton** *(Invited)*, High-throughput Computational Search for Strengthening Precipitates in Alloys, TMS Annual Meeting, Nashville, TN, USA (2/16)
30. **C. Wolverton** *(Invited)*, Assessing the Accuracy of DFT Formation Energies, TMS Annual Meeting, Nashville, TN, USA (2/16)
31. **S. S. Naghavi**, V. I. Hegde, C. Wolverton, "First-principles Co database: Energetics of binary Co alloys and compounds", American Physical Society, USA (3/15/16)
32. **O. L. Kafka**, C. Yu, J. A. Moore, W. K. Liu, "Multiscale fatigue modeling: NitTi and AM", Steel Research Group Annual Meeting, Evanston, IL, USA (3/21/16)
33. J. Gong, "ICME Design of Ni & Co Superalloys", 2016 Steel Research Group (SRG) Meeting, Evanston, IL, USA (3/21/16)

34. **C. Wolverton** *(Invited)*, American Chemical Society, Philadelphia, PA, USA (3/16)
35. **C. Wolverton** *(Invited)*, German Physical Society, Germany (3/16)
36. **A. Umantsev** *(Invited)* "Field Theory of Homogeneous Nucleation at Large Driving Forces" 20th Research Workshop on Nucleation Theory and Applications, Bogolubov Research laboratory, JINR, Dubna, Russian Federation (4/18/16)
37. **J. Thapa**, C. Gross, Y-W. Chung, M. J. Bedzyk. "High Throughput Combinatorial Studies of Co-based Alloys" International Conference on Metallurgical Coatings and Thin Films, San Diego, CA, USA (4/16)
38. **A. Umantsev** *(Invited)* "Nucleation at Large Driving Forces", Russian Academy of Sciences, Joint Institute for High Temperatures, Moscow, Russian Federation (5/26/16)
39. **A. Umantsev** *(Invited)* "Role of Internal Boundaries in the stability of Nanosystems" XV International Conference on Integranular and Interphase Boundaries in Materials, National University of Science and Technology, Moscow, Russian Federation (5/17/16)
40. **C. Wolverton** *(Invited)*, Department Colloquium, Univ. of Washington, Seattle, WA, USA (5/16)
41. **C. Wolverton** *(Invited)*, Department Colloquium, MIT, Boston, MA, USA (5/16)
42. **C. Wolverton** *(Invited)*, Department Colloquium, Johns Hopkins University, Baltimore, MD, USA (5/16)
43. **O. L. Kafka**, W. K. Liu, "First Steps in a predictive model for surface void nucleated fatigue", VII European Congress on Computational Methods in Applied Sciences and Engineering, Crete, Grece (6/5/16)
44. **A. Umantsev** *(Invited)* "Long-Period Stacking Fault Structures of Magnesium-Base Alloys", National University of Science and Technology, Moscow, Russian Federation (6/14/16)
45. **A. Umantsev** *(Invited)* "Nucleation at Large Driving Forces", Department of Statistical Physics, St. Petersburg State University, Russian Federation. (6/17/16)
46. **C. Wolverton** *(Invited)*, IU-MRS Meeting, Singapore (6/16)
47. **C. Wolverton** *(Invited)*, Next Generation Electrochemistry Summer School, UIC, Chicago, IL, USA (6/16)
48. **C. Wolverton** *(Invited)*, Electrochemical Society Annual Meeting, USA (6/16)
49. **A. Umantsev** The Fifth Anniversary of the Materials Genome Initiative, Accomplishments and Opportunities, The White House, Eisenhower Executive Office Building, Washington, DC, USA (8/2/16)
50. **M. Stan** *(Invited)*, "Bridging Scales in Modeling and Experimentation", The Modeling and Experimental Validation Summer School, ORNL, Oak Ridge, TN, USA (8/20/16)
51. **C. Wolverton** *(Invited)*, CAMD Summer School, Copenhagen, Sweden (8/16)
52. **C. Wolverton** *(Invited)*, American Chemical Society Fall Meeting, Philadelphia, PA, USA (8/16)
53. **C. Wolverton** *(Invited)*, IPAM Workshop, "Machine Learning meets Many Particle Problems", UCLA, CA, USA (8/16)
54. **M. Stan** *(Invited)*, P. Cristea., "Certainty and Uncertainty of Thermodynamic Data", RomPhysChem 16 Conference, Galati, Romania, (9/21/16)
55. **C. Wolverton** *(Invited)*, Vienna Young Researchers Workshop, Vienna, Austria (9/16)
56. **M. Stan** *(Invited)*, "Certainty and Uncertainty at High Temperatures", Structure and

Thermodynamics of Oxides at High Temperature (STOHT16) Conference, Univ. of California, Davis, CA, USA (10/21/16)

57. **C. Wolverton** *(Invited)*, Lorentz Center Workshop, "Open Databases Integration for Materials Design, Leiden, Netherlands (10/16)
58. **A. Umantsev** *(Invited)* The 3rd International Symposium on Long-Period Stacking Ordered Structure and Its Related Materials (LPSO 2016) Kyoto, Japan (12/4/16)

24.14 ASM

1. CMD Network e-newsletter article January edition, "Materials Genome Toolkit contest underway," 1/21/2016
2. CMD Network e-newsletter article March edition, "Deadline extended for Materials Genome Toolkit contest," 3/17/2016
3. CMD Network e-newsletter article May edition, "Judging underway in Materials Genome Toolkit competition," 5/19/2016
4. CMD Network e-newsletter article August edition, "Three schools win ASM Materials Genome Toolkits," 8/25/2016
5. ASM Materials Genome Toolkit winners (*Press Release*), 6/14/2016
6. Materials Genome Toolkit Program web post and application form: http://www.asminternational.org/web/guest/foundation/students/material-genome

25. Publications

1. Zhao H., Li X., Zhang Y., Schadler L. S., **Chen** W. , **Brinson** L. C., NanoMine: a material genome approach for polymer nanocomposites analysis and design, APL-Materials, vol 4: 053204, 2016. [DOI: 10.1063/1.4943679] *Partial Support*

2. Hassinger I., Li X., Zhao H., Xu H., Li Y., Krentz T., Huang Y., Schadler L. S., **Chen** W., **Brinson** L. C., Towards the Development of a Quantitative Tool for Predicting Dispersion of Nanocomposites Under Non-Equilibrium Processing Conditions, Journal of Materials Science, 51(9):4238-4249, 2016. [DOI: 10.1007/s10853-015-9698-1] *Partial Support*

3. Tchoua, R. B. , Chard K., **Audus** D., Qin J., **de Pablo** J., **Foster**, I, A Hybrid Human-computer Approach to the Extraction of Scientific Facts from the Literature, Procedia Computer Science, Volume 80, 386-397, 2016. [DOI:10.1016/j.procs.2016.05.338] *Primary Support*

4. Tchoua, R. B. , Chard K., **Audus** D., Qin J., **de Pablo** J., **Foster**, I, Blending Education and Polymer Science: Semiautomated Creation of a Thermodynamic Property Database, Journal of Chemical Education 93 (9), 1561-1568, 2016. [DOI: 10.1021/acs.jchemed.5b01032] *Primary Support*

5. Fox D., Rodriguez R. S., Devilbiss M. N. , **Woodcock** J. , Davis C. S. , Sinko R., **Keten** S., **Gilman** J. W. , Simultaneously Tailoring Surface Energies and Thermal Stabilities of Cellulose Nanocrystals Using Ion Exchange: Effects on Polymer Composite Properties for Transportation, Infrastructure, and Renewable Energy Applications, Applied Materials and Interfaces , 8, 27270-27281, 2016. [DOI:10.1021/acsami.6b06083] *Primary Support*

6. Xia, W., Song J., Hsu D., **Keten** S., Understanding the Interfacial Mechanical Response of Nanoscale Polymer Thin Films via Nanoindentation, Macromolecules, 49 (10), 3810-3817, 2016. [DOI: 10.1021/acs.macromol.6b0012] *Primary Support*

7. Xia, W., Song J., Hsu D., **Keten** S., Designing multi-layer graphene-based assem-

blies for enhanced toughness in nacre-inspired nanocomposites, Molecular Systems Design and Engineering, 1, 40-47, 2016. [DOI: 10.1039/C6ME00022C] *Partial Support*

8. Han, M., Wu, H., **Luijten**, E., Electric double layer of anisotropic dielectric colloids under electric fields, Eur. Phys. J. Special Topics 225, 685-698, 2016. [DOI: 10.1140/epjst/e2015-50316-9] *Primary Support*

9. Wu, H., Han, M., **Luijten** E., Dielectric Effects on the Ion Distribution near a Janus Colloid, Soft Matter, 2016. [DOI: 10.1039/c6sm01675h] *Primary Support*

10. Liu, X., Balla, I., Bergeron, H., Campbell, G. P., **Bedzyk**, M. J., **Hersam** M. C., Rotationally Commensurate Growth of MoS2 on Epitaxial Graphene, ACS Nano, 10, 1067-1075 (2016). [DOI: 10.1021/acsnano.5b06398] *Partial Support*

11. Liu, X., Balla, I., Bergeron, **Hersam** M. C., Point Defects and Grain Boundaries in Rotationally Commensurate MoS_2 on Epitaxial Graphene, Journal of Physical Chemistry C, 120, 20798 (2016). [DOI: 10.1021/acs.jpcc.6b02073] *Partial Support*

12. Ren X., **Singh** A. K., Fang, L., Kanatzidis, M. G., **Tavazza**, F., **Davydov** A. V., **Lauhon**, L. J., Atom Probe Tomography Analysis of Ag Doping in 2D Layered Material $(PbSe)_5(Bi_2Se_3)_3$, Nano Letters, 16, 6064-6069 (2016). [DOI: 10.1021/acs.nanolett.6b02104] *Primary Support*

13. Ryder R., Wood, J. D. , Wells, S. A., Yang, Y. , Jariwala, D. , **Marks**, T. J. , Schatz, G. C., **Hersam**, M. C., Covalent functionalization and passivation of exfoliated black phosphorus via aryl diazonium chemistry, Nature Chemistry, 8, 597 (2016). [DOI: 10.1038/nchem.2505] *Partial Support*

14. Ren, J., Ocola, L. E., Divan, R., Czaplewski, D. A., Segal-Peretz, T., Xiong, S., **Kline**, R. J., Arges, C. G., **Nealey**, P. F., Post-Directed-Self-Assembly Membrane Fabrication for in Situ Analysis of Block Copolymer Structures. Nanotechnology, 27, 435303 (2016). [DOI: 10.1088/0957-4484/27/43/435303] *Primary Support*

15. Suh, H. S., Chen, X., Rincon-Delgadillo, P. A., Jiang, Z., Strzalka, J., Wang, J., Chen, W., Gronheid, R., de **Pablo**, J. J., Ferrier, N., Doxastakis, M., **Nealey** P. F., Characterization of the Shape and Line-Edge Roughness of Polymer Gratings with Grazing Incidence Small-Angle X-Ray Scattering and Atomic Force Microscopy. J. Appl. Crystallogr. 49, 823-834 (2016). [DOI: 10.1107/S1600576716004453] *Partial Support*

16. Segal-Peretz, T., Zhou, C., Ren, J., Dazai, T., Ocola, L. E., Divan, R. N. S., **Nealey**, P. F., Three Dimensional Assembly in Directed Self-Assembly of Block Copolymers. J. Photopolym. Sci. Technol. 29, 653-657 (2016) [DOI: 10.2494/photopolymer.29.653] *Partial Support*

17. Ramirez-Hernandez A., Peters B. L., Schneider L., Andreev M., Schieber J. D., Muller M., **de Pablo** J. J. A multi-chain polymer slip-spring model with fluctuating

number of entanglements: Density fluctuations, confinement, and phase separation. The Journal of Chemical Physics. 46(1) 014903 (2017) [DOI: 10.1063/1.4972582]

18. **Jaeger**, H. M.; **de Pablo**, J. J., Perspective: Evolutionary design of granular media and block copolymer patterns, APL Materials, 4(5) 053209 (2016) [DOI: 10.1063/1.4948270] *Primary Support*

19. M. Z. Miskin, G. S. Khaira, J. J. **de Pablo**, and H. M. **Jaeger**, Turning Statistical Physics Models Into Materials Design Engines, Proceedings of the National Academy of Sciences 113, 34-39 (2016). [DOI: 10.1073/ pnas.1509316112] *Partial Support*

20. L. K. Roth, H. M. **Jaeger**, Optimizing Packing Fraction in Granular Media Composed of Overlapping Spheres, Soft Matter 12, 1107-1115 (2016). [DOI: 10.1039/c5sm02335a] *Partial Support*

21. Smith, J., Xiong, W., Yan, W., Lin, S., Cheng, P., Kafka, O.L., Wagner, G.J., **Cao**, J., **Liu**, W.K. "Linking process, structure, property, and performance for metal-based additive manufacturing: computational approaches with experimental support", Computational Mechanics (2016) [DOI: 10.1007/s00466-015-1240-4] *Partial Support*

22. Bennett, J. L., Dudas, R. J., **Cao**, J., Ehmann, K. and Hyatt, G., "Control of Heating and Cooling for Direct Laser Deposition Repair of Cast Iron Components", Int. Conf. Flexible Automaton, 2016. IEEE [DOI: 10.1109/ISFA.2016.7790166] *Primary Support*

23. Srivastava, S., **Tirrell**, M. V., "Polyelectrolyte Complexation" Advances in Chemical Physics, 161, 499-544 (2016). [DOI: 10.1002/9781119290971.ch7] *Primary Support*

24. Srivastava, S., Andreev M., Levi A., Goldfeld D., Mao S., **Prabhu** V. M., **de Pablo** J. J., **Tirrell** M. V., "Gel Phase Formation in Dilute Triblock Copolyelectrolyte Complexes" Nature Communications, 7, 14131 (2016). [DOI: 10.1038/ncomms14131] *Primary Support*

25. Zhou, N., Dudnik A. S., Li T. I. N. G., Manley E. F., Aldrich T. J., Guo P., Liao H-C., Chen Z., Chen, L. X., Chang R. P. H., Facchetti A., **Olvera de la Cruz** M., **Marks** T. J., "All-Polymer Solar Cell Performance Optimized via Systematic Molecular Weight Tuning of Both Donor and Acceptor Polymers" Journal of the American Chemical Society, 138, 1240-1251, (2016) [DOI: 10.1021/jacs.5b10735] *Partial Support*

26. G. Kocher, N. Ofori-Opoku, N. Provatas, Incorporating noise quantitatively in the phase field crystal model via capillary fluctuation theory", PRL, 117(22), 220601, (2016) [DOI: 10.1103/PhysRevLett.117.220601] *Partial Support*

27. Blaiszik, B., Chard K., Pruyne, J., Ananthakrishnan, R., **Tuecke** S., **Foster**., I. "The Materials Data Facility: Data Services to Advance Materials Science research" JOM 68, 8: 2045-2052 [DOI: 10.1007/s11837-016-2001-3]

28. Rocks J. W., Pashine N., Bischofberger I., Goodrich, C. P., Liu A. J., **Nagel**, S.

R. "Designing allostery-inspired response in mechanical networks" Proc. National Academy of Sciences 114(10), 2520-2525, [DOI: 10.1073/pnas.1612139114] *Partial Support*

29. Poulsen, S. O., **Voorhees**, P. W., "Early stage phase separation in ternary alloys: A test of continuum simulations" Acta Mater. 113 90-108 (2016) [DOI: 10.1016/j.actamat.2016.04.054] *Partial Support*

30. Jokisaari, A. M., **Voorhees** P. W., **Guyer** J.E., **Warren** J., **Heinonen** O.G. "Benchmark problems for numerical implementations of phase field models" Comp. Mater. Science. 126 139-151 (2017) [DOI: 10.1016/commatsci.2016.09.022] *Primary Support*

31. Zhang J., Poulsen S. O., Gibbs J. W., **Voorhees**, P. W., Poulsen, H. F., "Determining material parameters using phase-field simulations and experiments" Acta Materiala, 129, 229-238 (2017) [DOI: 10.1016/j.actamat.2017.02.056] *Partial Support*

32. Zhao D., Wu Q., Cai Z., Zheng T., Chen W., Lu J., **Yu**, L. "Electron Acceptors Based on π-Substituted Perylene Diimide (PDI) for Organic Solar Cells", Chemistry of Materials 28 (4), 1139-1146 (2016) [DOI: 10.1021/acs.chemmater.5b04570] *Partial Support*

33. Wu Q., Zhao, D., Schneider, A. M., Chen, W., **Yu**, L., "Covalently Bound Clusters of Alpha-Substituted PDI-Rival Electron Acceptors to Fullerene for Organic Solar Cells", Journal of the American Chemical Society, 138 (23), 7248-7251 (2016) [DOI: 10.1021/jacs.6b03562] *Partial Support*

34. Goldey M., Reid D., **de Pablo** J., **Galli** G. "Planarity and multiple components promote organic photovoltaic efficiency by improving electronic transport" Phys. Chem. Chem. Phys. 18, 31388-31399 (2016) [DOI: 10.1039/C6CP04999K] *Primary Support*

35. Melkonyan, F. S.; Zhao, W.; Drees, M.; Eastham, N. D.; Leonardi, M. J.; Butler, M. R.; Chen, Z. H.; Yu, X. G.; Chang, R. P. H.; Ratner, M. A.; Facchetti, A. F.; **Marks**, T. J.: Bithiophenesulfonamide Building Block for pi-Conjugated Donor-Acceptor Semi-conductors. J. Am. Chem. Soc. 138, 6944-6947 (2016) [DOI: 10.1021/jacs.6b03498] *Primary Support*

36. Eckstein, B. J., Melkonyan, F. S., Zhou, N., Manley, E. F., Smith, J.; Timalsina, A., Chang, R.P.H., Chen, L.X., Facchetti, A., **Marks**, T.J., Buta-1,3-diyne Based π-Conjugated Polymers for Organic Transistors and Solar Cells, Macromolecules, 50 (4), pp 1430-1441 (2017) *Partial Support*

37. **Agrawal**, A., **Choudhary**, A., "Perspective: Materials informatics and big data: Realization of the *fourth paradigm* of science in materials science", APL Materials, vol. 4, no. 053208, 1-10, (2016) [DOI: 10.1063/1.4946894] *Partial Support*

38. **Agrawal**, A., **Choudhary**, A., "A Fatigue Strength Predictor for Steels Using

Ensemble Data Mining," in Proceedings of 25th ACM International Conference on Information and Knowledge Management (CIKM), 2497-2500 (2016) [DOI: 10.1145/2983323.2983343] *Primary Support*

39. **Agrawal,** A., Meredig B., **Wolverton** C., **Choudhary**, A., "A Formation Energy Predictor for Crystalline Materials Using Ensemble Data Mining", in Proceedings of IEEE International Conference on Data Mining (ICDM), 1276-1279 (2016) [DOI: 10.1109/ICDMW.2016.0183] *Primary Support*

40. Furmanchuk A.,**Agrawal**, A., **Choudhary**, A., "Predictive analytics for crystalline materials: Bulk modulus," RSC Advances, 6, (97), 95246-95251 (2016) [DOI: 10.1039/C6RA19284J] *Partial Support*

41. Ward L., **Agrawal** A., **Choudhary** A., **Wolverton** C., "A General-Purpose Machine Learning Framework for Predicting Properties of Inorganic Materials" npj Computational Materials, 2 (16028) (2016) [DOI: 10.1038/npjcompumats.2016.28] *Primary Support*

42. Ward L., **Wolverton** C., "Atomistic calculations and materials informatics: A review." Curr. Opin. Solid State Mater. Sci. (2016). [DOI: 10.1016/j.cossms.2016.07.002] *Primary Support*

43. Liu R., Ward L., **Wolverton** C., **Agrawal** A., Liao W.-K. , **Choudhary**, A., "Deep Learning for Chemical Compound Stability Prediction", Proceedings of ACM SIGKDD Workshop on Large-scale Deep Learning for Data Mining (DL-KDD), 2016. To appear. [DOI: Not yet available] *Primary Support*

44. Bostanabad, R., **Chen** W., Apley, D. W. "Characterization and reconstruction of 3D stochastic microstructures via supervised learning" Journal of Microscopy (2016) [DOI: 10.1111/jmi.12441] *Partial Support*

45. Hill, J., Mulholland, G., Persson, K., Seshadri, R., **Wolverton**, C., Meredig, B., "Materials science with large-scale data and informatics: Unlocking new opportunities" MRS Bull. 41, 399-409 (2016) [DOI: 10.1557/mrs.2016.93] *Partial Support*

46. **Saal**, J., **Wolverton**, C., "Energetics of antiphase boundaries in $\gamma' Co_3(Al,W)$-based superalloys. Acta Materialia, 103 57-62. (2016) [DOI: 10.1016/j.actamat.2015.10.007] *Primary Support*

47. Zhou J., Odqvist J., Agren J., Ruban A., Thuvander M., Xiong W., **Olson** G. B., Hedstrom P., "Direct atom probe tomography observations of concentration fluctuations in Fe-Cr solid solution", Scripta Materialia, 98, 13-15 (2015) [DOI: 10.1016/j.scriptamat.2014.10.035] *No CHiMaD Support*

48. Xiong W., **Olson** G. B.,"Integrated Computational Materials Design for High-Performance Alloys", MRS Bulletin, 40 (12) 1035-1044 (2015) [DOI: 10.1557/mrs.2015.273] *Primary Support*

49. Yan, J-Y., **Olson** G. B, "Computational Thermodynamics and Kinetics of Displacive Transformations in Titanium-based Alloys," Journal of Alloys and Compounds 673 (2016) [DOI: 10.1016/j.jallcom.2016.02.251] *No CHiMaD Support*

50. Xiong W., **Olson** G. B., "Cybermaterials: Materials by Design and Accelerated Insertion of Materials", npj Computational Materials 2 15009-15032 (2016) [DOI:10.1038/npjcompumats.2015.9] *Primary Support*

51. Wang, Z, **Chen**, W., "Confidence-based Adaptive Extreme Response Surface for Time-Variant Reliability Analysis under Random Excitation" Structural Safety, 64, 76-86 (2017) [DOI: 10.1016/j.strusafe.2016.10.001] *Primary Support*

52. Wang, Z, **Chen**, W., "Time-Variant Reliability Assessment through Equivalent Stochastic Process Transformation", Reliability Engineering & System Safety, 152, 166-175, (2016) [DOI: 10.1016/j.ress.2016.02.008] *Primary Support*

53. Naghavi S. S., Hegde V. I., Saboo, A., **Wolverton** C. "First-principles Co database: Energetics of binary Co alloys and compounds" Acta Materialia (in press, 2016) [DOI: 10.1016/j.actamat.2016.10.065] *Primary Support*

54. Moore J. A., **Frankel** D., Prasannavenkatesan R., Domel A. G., **Olson** G. B., **Liu** W. K., "A crystal plasticity-based study of the relationship between microstructure and ultra-high-cycle fatigue life in nickel titanium alloys", International Journal of Fatigue, 91 (1), 183-194. (2016) [DOI: 10.1016/j.ijfatigue.2016.06.006] *Primary Support*

55. Jia Z., **Liu** W. K., "Rate-dependent stress evolution in nanostructured Si anodes upon lithiation", Applied Physics Letters, 109 (16), [DOI: 10.1063/1.4964515] *Primary Support*

56. Jia Z., **Liu** W. K., "Analytical model on stress-regulated lithiation kinetics and fracture of Si-C yolk-shell anodes for lithium-ion batteries", Journal of the Electrochemical Society, 163 (6), A940-A946 (2016) [DOI: 10.1149/2.0601606jes] *Primary Support*

57. Uzunov D., **Umantsev**, A. "Equilibrium Fluctuations in a Metastable State of a Ginzburg-Landau System", Physica A 448, 283-299 (2016) *Primary Support* [DOI: 10.1016/ j.physa.2015.12.098]

58. **Umantsev** A., "Lifetime of Metastable States in a Ginzburg-Landau System: Numerical Simulations at Large Driving Forces", Phys. Rev. E. 93, 002800 (2016) [DOI: 10.1103/PhysRevE.93.042806] *Primary Support*

59. **Umantsev**, A., Ode, M., "Formation of Long-Period Stacking Fault Structures in Magnesium Alloys", Comp. Mater. Sci 124, 173-182 (2016) [DOI: 10.1016/ j.commatsci.2016.07.035] *Primary Support*

60. Sauza D. J., Bocchini, P. J., **Dunand** D. C., **Seidman** D. N., "Influence of ruthenium

on microstructural evolution in a model Co-Al-W superalloy", Acta Materialia, 117(15), 135-145, (2016) [DOI: 10.1016/j.actamat.2016.07.014] *Primary Support*

61. Liu, Q., Coakley, J., **Seidman** D. N., **Dunand** D. C., "Precipitate Evolution and Creep Behavior of a W-Free Co-based Superalloy", Metall. and Mat Trans A (2016) [DOI: 10.1007/ s11661-016-3775-1] *Primary Support*

62. Cordoba, A., Hinckley, D., Lequieu, J., **de Pablo**, J. J., "A Molecular View of the Dynamics of dsDNA Packing inside Viral Capsids in the Presence of Ions, Biophysical Journal, (2017) [DOI: 10.1016/j.bpj.2017.02.015] *Primary Support*

CHiMaD

NORTHWESTERN UNIVERSITY

THE UNIVERSITY OF CHICAGO

Argonne NATIONAL LABORATORY

QuesTek INNOVATIONS LLC

FAYETTEVILLE STATE UNIVERSITY

ASM INTERNATIONAL

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce