CMEDE

CENTER FOR
MATERIALS IN EXTREME
DYNAMIC ENVIRONMENTS

2017 HIGHLIGHTS

WHAT IS CMEDE?

THE CENTER FOR MATERIALS IN EXTREME DYNAMIC ENVIRONMENTS IS A MULTI-INSTITUTION COLLABORATIVE RESEARCH CENTER LOCATED WITHIN THE HOPKINS EXTREME MATERIALS INSTITUTE AT JOHNS HOPKINS UNIVERSITY.

The Center brings together academia, government, and industry to advance the state of the art for materials in extreme dynamic environments.

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CONSORTIUM MANAGEMENT COMMITTEE

FROM THE CMEDE DIRECTOR:

Welcome to the third edition of the Center for Materials in Extreme Dynamic Environments (CMEDE) highlights. 2017 has been an exciting year for CMEDE! We have continued our extensive collaborative research activities across all four materials groups (ceramics, composites, metals and polymers) and have made exciting scientific advances as we cultivate the future materials-by-design workforce.

2017 was filled with significant events for the MEDE program. In February, we underwent a mid-cycle review with the ARL Chief Scientist, ARO Director, and the Deputy Chief Scientist of ASA(ALT). They were very pleased at the progress of the MEDE Collaborative Research Alliance (CRA) and provided excellent recommendations for future directions. Additionally, due to the importance of MEDE research, we are grateful that there has been significant Congressional interest in our program.

Our academic programs also benefitted from additional support from the U.S. Army. In 2017, MEDE was awarded an Army Educational Outreach Program, Undergraduate Research and Apprenticeship Program grant. This grant provided six summer internships that were conducted at various MEDE consortium universities. This program joins our Extreme Science Internship program with Morgan State University in helping develop the next generation of scientists and engineers.. I appreciate the investment in time by both the MEDE principal investigators and mentors in these programs.

As always, we are thankful for the continued support from the U.S. Army and the Department of Defense, as well as the support within the Enterprise for Multiscale Research of Materials and the partners in the MEDE CRA, without whom none of this would be possible.

As we move forward into 2018, I am excited to see our advances in developing an integrated, materials-by-design capability transition towards protection materials that benefit the U.S. Army.

K.T. RAMESH
Director, CMEDE

Alonzo G. Decker Jr. Professor
of Science and Engineering

Professor, Department of
Mechanical Engineering, Earth
and Planetary Sciences, Materials
Science and Engineering
Johns Hopkins University

JOHN H. BEATTY
Cooperative Agreement Manager
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California Institute of Technology

JOHN W. GILLESPIE, JR.
Donald C. Phillips Professor of Civil and Environmental Engineering

Professor, Mechanical Engineering, Materials Science and Engineering
University of Delaware

RICHARD HABER
Professor, Materials Science and Engineering
Rutgers University

ABOUT US

In 2010, two National Research Council boards established a committee to examine opportunities in protection materials science and technology for future Army applications. This committee recommended that the Department of Defense establish an initiative for protection materials by design. This initiative would include a combination of computational, experimental, and materials testing, characterization, and processing research to be conducted by academia, government, and industry.

In response to the committee's recommendation, in April 2012 the Army Research Laboratory (ARL) established a framework to integrate the Army's multiscale basic research in materials into one coordinated enterprise. Called the Enterprise for Multiscale Research of Materials (EMRM), the focus of the program is to develop a materials-by-design capability for the U.S. Army using validated multiscale and multidisciplinary modeling capabilities to predict material structure, properties, and performance.

Called the Enterprise for Multiscale Research of Materials (EMRM), the focus of the program is to develop a materials-by-design capability for the US Army using validated multiscale and multidisciplinary modeling capabilities to predict material structure, properties, and performance.

The EMRM enables ARL to coordinate its in-house activities with extramural research efforts. The EMRM is organized into four major areas: protection materials, energetic materials, electronic materials, and cross-cutting computational science.

To launch the protection materials research component of EMRM, ARL competitively awarded and then signed the Materials in Extreme Dynamic Environments cooperative research agreement with Johns Hopkins University (JHU), the California Institute of Technology (Caltech), the University of Delaware (Delaware) and Rutgers University. The agreement allowed JHU, which is the lead research organization within the consortium of university and research partners, to establish the Center for Materials in Extreme Dynamic

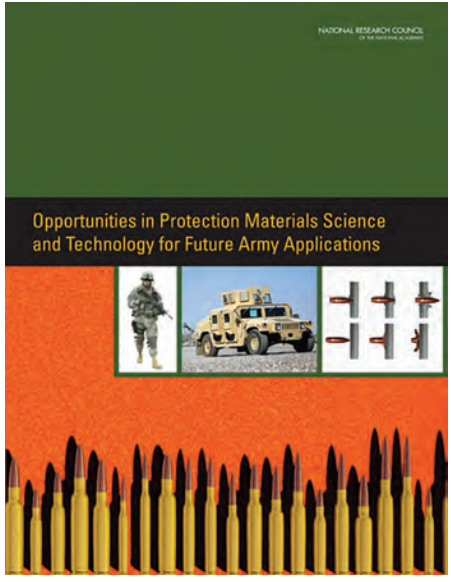


Figure 1: *National Research Council report*

Environments, or CMEDE. CMEDE is a center within the Hopkins Extreme Materials Institute, and focuses on advancing the fundamental understanding of materials in high-stress and high-strain-rate regimes, with the goal of developing a materials-by-design capability for these extreme environments. This 10-year agreement, valued up to $90 million, represents a significant investment and demonstrates the importance of the design of protection materials to the U.S. Army.

The MEDE program also supports the Presidential Materials Genome Initiative (MGI) for Global Competitiveness. Established in June 2011, MGI aims to double the speed at which materials are discovered, developed, and deployed. The MEDE program represents one of the Department of Defense's largest investments in extramural basic research in support of the MGI.

"The real holy grail of technologies that I'm trying to find is material...is the armor itself."

- GENERAL MARK MILLEY

39th Chief of Staff for the U.S. Army at a National Press Club Luncheon

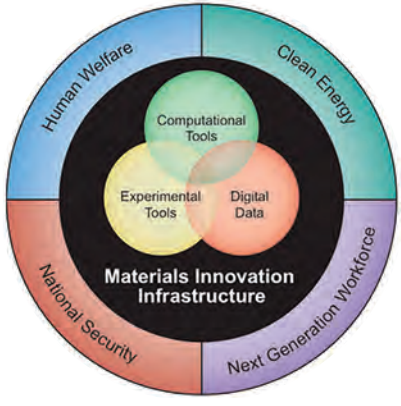


Figure 2: *Materials Genome Initiative: MEDE focuses on developing the experimental and computational tools needed to develop protection materials for national security.*

ORGANIZATION

The MEDE Collaborative Research Alliance (CRA) is composed of a consortium of university and research partners and the Army Research Laboratory. The MEDE consortium members include:

- **Johns Hopkins University (Lead)**
- **California Institute of Technology**
- **University of Delaware**
- **Rutgers University**
- **Drexel University**
- **Ernst Mach Institut**
- **Morgan State University**
- **New Mexico Institute for Mining and Technology**
- **North Carolina Agricultural and Technical State University**
- **Purdue University**
- **Southwest Research Institute**
- **University of North Carolina at Charlotte**
- **University of Texas at San Antonio**

Additionally, through government agreements, the MEDE CRA collaboratively works with the Defence Science and Technology Laboratory of the United Kingdom.

The MEDE CRA is composed of a consortium of university and research partners and the Army Research Laboratory. It also works internationally with the Defence Science and Technology Laboratory of the United Kingdom.

Johns Hopkins University

New Mexico Tech
Science • Engineering • Research • University

Caltech

North Carolina Agricultural and Technical State University

University of Delaware

Purdue University

Rutgers

SwRI

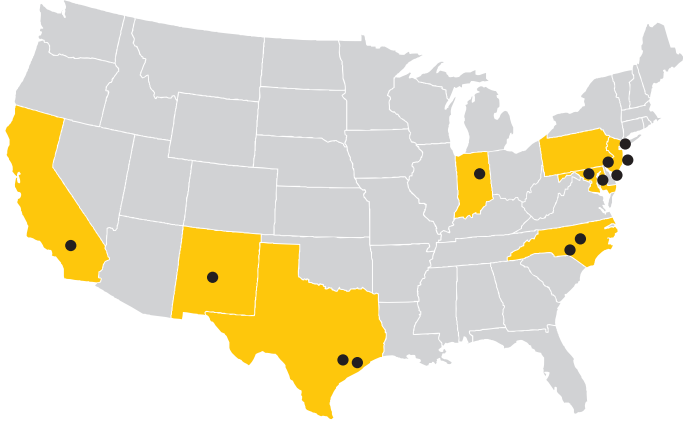
Drexel University

UNC Charlotte

Morgan State University

UTSA

ARL



United Kingdom

[dstl]

Germany

Fraunhofer EMI

Figure 3: *MEDE Collaborative Research Alliance*

STRUCTURE

- The CMEDE Director is located within CMEDE at Johns Hopkins University, the lead research organization for the MEDE CRA.
- The MEDE Science Advisory Board complements ARL's Technical Advisory Board. It provides important scientific insight, oversight, and expertise to the CMEDE consortium. The Board reports to the CMEDE Director.
- The Consortium Management Committee (CMC) is composed of a senior representative from the four major consortium partners and the ARL Cooperative Agreement Manager. The CMC is the final decision authority for the MEDE CRA.
- A Collaborative Materials Research Group (CMRG) coordinates all research activities for each material type. Each CMRG is co-led by a consortium principal investigator and an ARL researcher.
- Within each CMRG, there are multiple technical areas, separated by scale or mechanism. The CMRGs are highly integrated with a consortium PI and an ARL researcher co-leading each major effort.

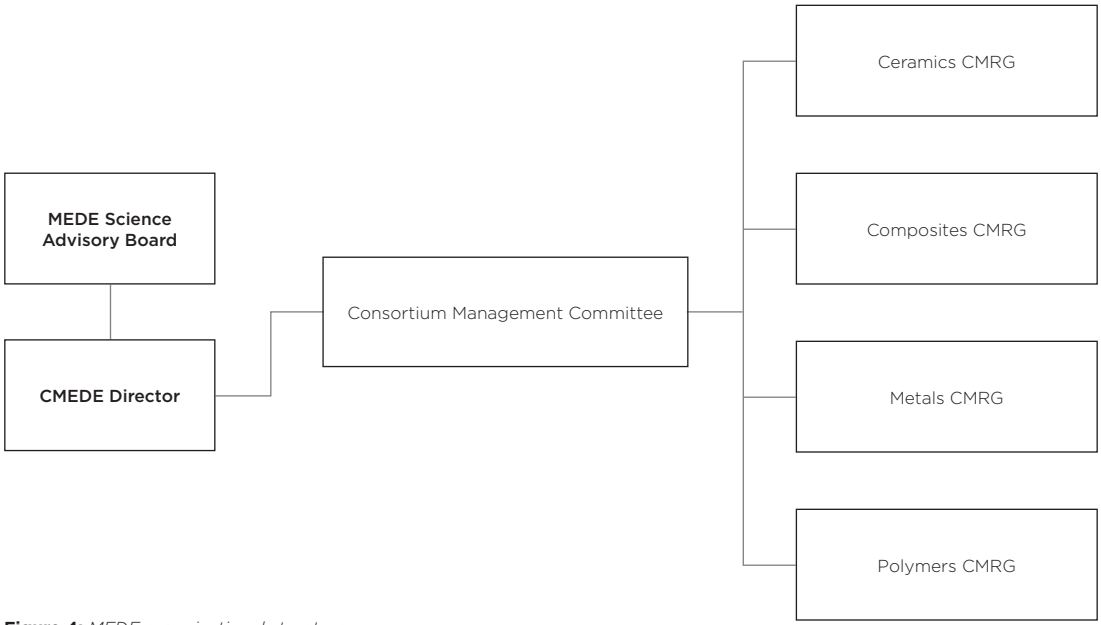


Figure 4: *MEDE organizational structure*

From left: Prof. Marc Meyers, Dr. Donald Shockey, Prof. Horacio Espinosa, Dr. Douglas Templeton.
Not shown: Prof. Irene Beyerlein, Prof. Rodney Clifton, Prof. David McDowell, Prof. Steven McKnight, Prof. Anthony Rollett, Prof. Thomas Russell, Prof. Susan Sinnott, Prof. Nancy Sottos.

MEDE SCIENCE ADVISORY BOARD MEMBERS

Dr. Donald Shockey
SRI International (Chair)

Professor David McDowell
Georgia Institute of Technology

Professor Thomas Russell
University of Massachusetts Amherst

Professor Irene Beyerlein
University of California, Santa Barbara

Professor Steve McKnight
Virginia Polytechnic Institute

Professor Susan Sinnott
Pennsylvania State University

Professor Rodney Clifton
Brown University

Professor Marc Meyers
University of California, San Diego

Professor Nancy Sottos
University of Illinois at Urbana-Champaign

Professor Horacio Espinosa
Northwestern University

Professor Anthony Rollett
Carnegie Mellon University

Dr. Douglas Templeton
DWT Consulting

RESEARCH STRATEGY

The objective of the MEDE program is to develop the technical and workforce capability to design, create, and optimize novel material systems that exhibit revolutionary performance in extreme dynamic environments. Achieving this objective requires a new paradigm for materials research and workforce development. One cannot use the classical materials science structure-properties-performance approach because path-dependent and time-dependent failure processes are involved in these dynamic environments, and optimal solutions may not exist in the traditional design space. Instead, we must design with knowledge of the dynamic failure processes (mechanisms) that are involved in the actual application.

The objective is not necessarily to produce a specific material system that is optimized for a specific range of applications, but rather to produce a way of thinking that will allow the design of lightweight protective material systems that can be used for extreme dynamic environments.

To achieve the MEDE program objectives, research activities are focused on a materials-by-design process involving a canonical model and a mechanism-based strategy as shown in Figure 5. We have established a canonical model for each model material under investigation. A canonical model is defined as: "A simplified description of the system or process, accepted as being accurate and authoritative, and developed to assist calculations and predictions."

Typically such a canonical model defines key variables and their ranges, defines critical mechanisms, and then prioritizes the variables and mechanisms. Beginning with a canonical model allows a large group of researchers to ensure that efforts are relevant in terms of both science and application.

Once the canonical description is established, researchers can then proceed with the mechanism-based strategy. Researchers seek to see the mechanisms during the extreme dynamic event, to understand them through multiscale models, and to control them through synthesis and processing. Understanding the mechanisms through multiscale models provides the capability to define integrative experiments and to test the coupling of mechanisms. This information leads to validated models and codes, which feed back into the canonical model, by transitioning into Department of Defense (DoD) and Department of Energy (DoE) codes. Similarly, controlling the mechanism through synthesis and processing leads to newly designed materials for the canonical environment. Industry helps to determine the scale-up feasibility of these newly designed materials, which are then fed back to the experiments in the canonical modeling effort.

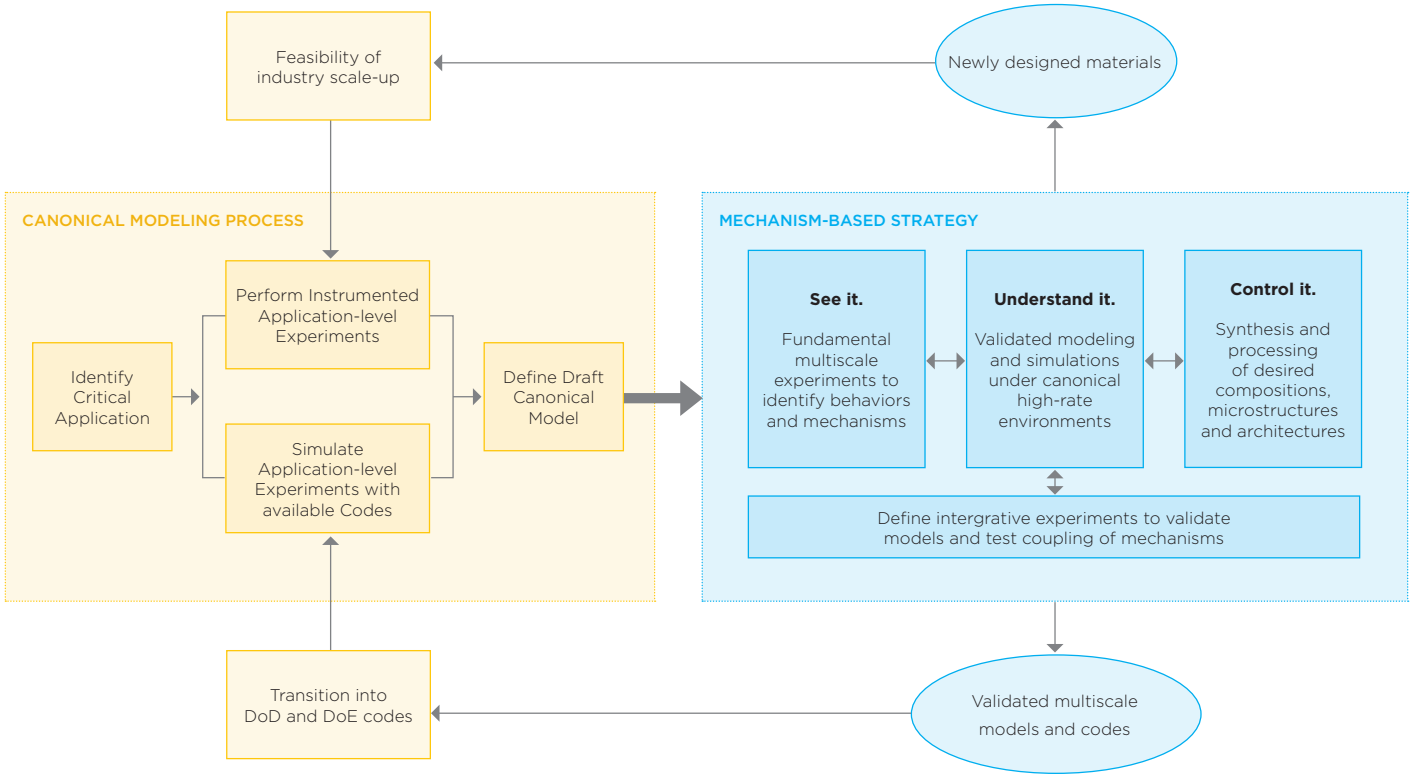


Figure 5: *Overall design strategy for protection materials. Left hand boxes are driven by ARL, while right hand boxes are driven by the MEDE Consortium.*

RESEARCH ACTIVITIES

The MEDE program examines one model material in each of the following four material classes: ceramics, composites, metals, and polymers. The discoveries and insights developed can be used for other materials in the same class.

Ceramics: Boron Carbide

Boron carbide is the model material for the Ceramics CMRG because it has the unrealized potential of dramatic improvements in ballistic performance for vehicular protection at very low weight. The Ceramics CMRG seeks to understand and control the dynamic failure processes in this protective ceramic material and to improve its dynamic performance by controlling mechanisms at the atomic and microstructural levels through multiscale modeling, advanced powder synthesis, control of polytypes, and microstructural improvements.

Application: Boron carbide is one of the component materials used to protect soldiers and military vehicles from blast and ballistic threats.

Composites: S-2 Glass/Epoxy

Composite materials subjected to dynamic loads are essential examples of high performance systems in the conventional sense. In order to focus on the complexities raised by the interfaces and architectures, S-2 Glass/Epoxy is the model system for the Composites CMRG. The Composites CMRG develops the fundamental understanding of the role of interfaces, component interactions, and composite architecture over the full range of length scales and time scales that are manifested in the system during the dynamic event.

Application: S-2 Glass/Epoxy provides a strong, structural backing system to support protective plates for military vehicles.


Photo: Jay Gould, MICA


Photo: Jay Gould, MICA


Photo: Jay Gould, MICA

Metals: Magnesium

The magnesium alloy system is the model material for the Metals CMRG because it is the lightest-weight structural metal that offers the potential of approaching steel-like ballistic performance while using conventional low-cost and time-tested processing techniques. We are enhancing the dynamic performance of this hexagonally-close-packed metal using experimentally validated modeling and alloy design to control dynamic strengthening and failure mechanisms, including deformation twinning.

Application: The U.S. Army's Stryker vehicle incorporates magnesium in its structure. In comparison to steel, magnesium offers the potential for a lightweight metal system that could enhance the deployability and protection of military vehicles.

Polymers: UHMWPE

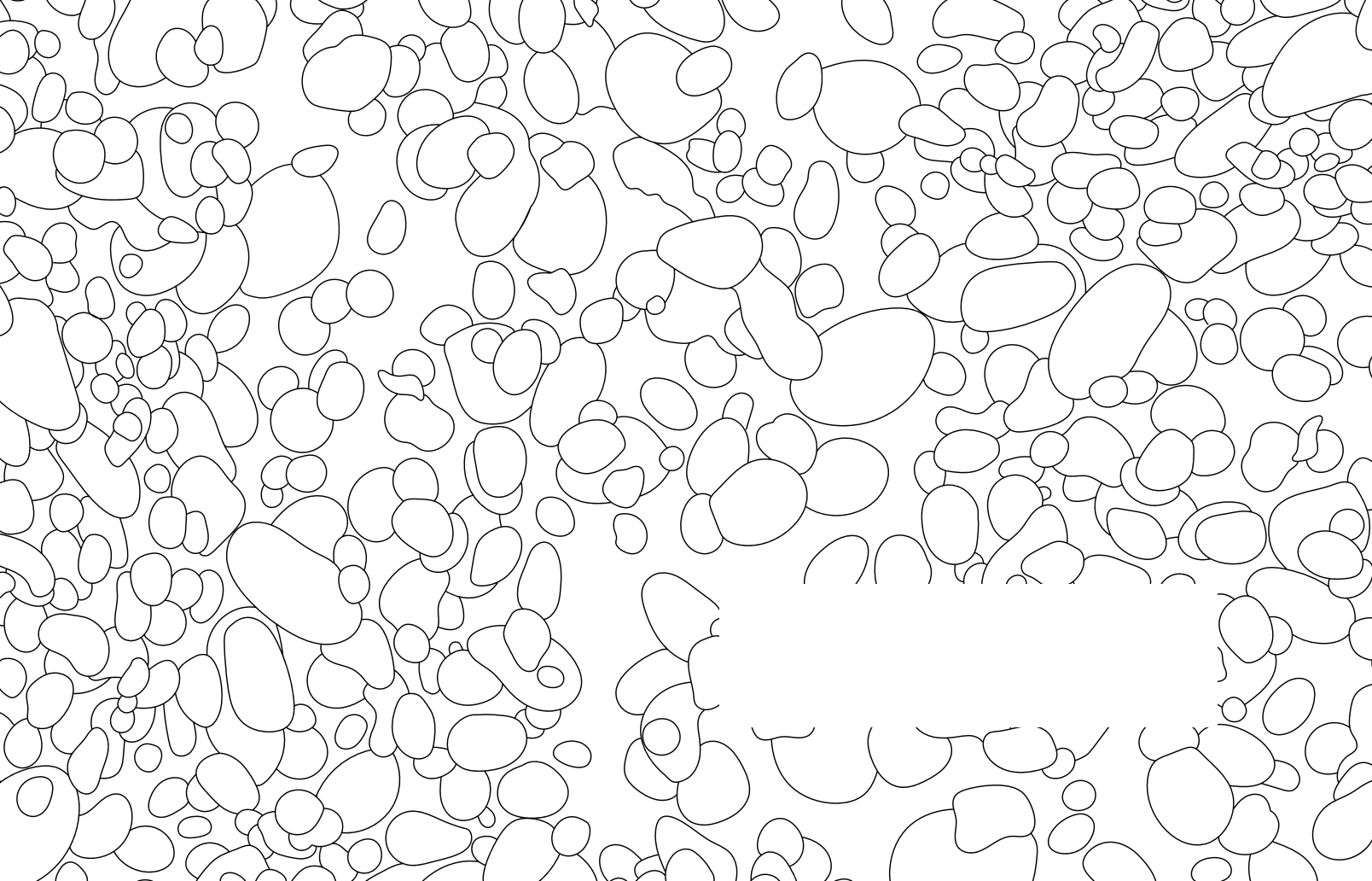
Polyethylene is the model system for the Polymers CMRG because of the potential for significant improvement in its mechanical properties. Ultra High Molecular Weight Polyethylene (UHMWPE) is used in a wide variety of military applications in both tape and fiber forms, but its tensile strength remains an order of magnitude below the theoretical value. The Polymers CMRG seeks to determine the roles of atomic scale defects, chain length, degree and length scale of crystallinity in determining and limiting the mechanical response under extreme dynamic conditions.

Application: UHMWPE shows tremendous promise for the next generation of helmets and body protection for soldiers.

CMEDE RESEARCH ACTIVITIES ADDRESS THE FOLLOWING FIVE CORE ELEMENTS:

- **Advanced Experimental Techniques:** developing experimental methodologies to interrogate and characterize the in-situ materials response to extreme dynamic environments at critical length and time scales.
- **Modeling and Simulation:** developing computational approaches to predict the materials response to extreme dynamic environments at critical length and time scales.
- **Bridging the Scales:** developing physical and mathematical constructs necessary to bridge critical length and time scales.
- **Material Characteristics and Properties at Multiple Scales:** utilize existing and novel experimental methodologies to identify the comprehensive set of material characteristics, microstructural features, and dynamic properties that govern high rate deformation and failure phenomena, and to validate computational approaches in order to bridge the characteristic length and time scales.
- **Synthesis and Processing:** incorporate research discoveries to enable the synthesis of novel materials and the processing of final products with critical material characteristics and resulting properties.

Artistic rendering of the atomic-level view of boron carbide as seen through a transmission electron microscope.



CERAMICS

Consortium Lead - Prof. Richard Haber (Rutgers)

ARL Lead - Dr. Jerry LaSalvia

Ceramics CMRG

CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Nitin Daphalapurkar, JHU

Dr. Vladislav Domnich, Rutgers

Prof. William Goddard, Caltech

Prof. Lori Graham-Brady, JHU

Prof. Rich Haber, Rutgers

Prof. Kevin Hemker, JHU

Prof. Todd Hufnagel, JHU

Prof. K.T. Ramesh, JHU

ARL COLLABORATORS

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Dr. Richard Becker

Dr. Kristopher Behler

Dr. Shawn Coleman

Dr. George Gazonas

Dr. Efrain Hernandez

Dr. Jerry LaSalvia

Mr. Brian Leavy

Dr. Jonathan Ligda

Dr. Bryan Love

Dr. James McCauley

Dr. Jason McDonald

Dr. Chris Meredith

Dr. Sikhanda Satapathy

Dr. Brian Schuster

Dr. Jeffrey Swab

Dr. Jennifer Synowczynski-Dunn

Dr. DeCarlos Taylor

Dr. Andrew Tonge

Dr. Mark Tschopp

Dr. Scott Walck

CONSORTIUM RESEARCH TASKS

- Characterization of Deformation Mechanisms and Amorphization in Boron Carbide (Haber and Domnich, Rutgers)
- Characterization of Defects and In Situ Visualization of Fracture in Boron Carbide (Hufnagel and Ramesh, JHU)
- Control of Inelastic Mechanisms in Boron Carbide Through Processing (Haber, Rutgers)
- Crack Coalescence, Comminution and Granular Flow of Highly Damages Ceramics (Graham-Brady and Ramesh, JHU)
- Extension of the First Principles Based ReaxFF Multiscale Simulation Technology Developed in MEDE-I to Full Scale Multigrain and Microalloying to Optimize Strength and Ductility in MEDE-II (Goddard, Caltech)
- High-Rate Characterization, Granular Flow and Amorphization in Boron Carbide Materials (Ramesh, JHU)
- Integrated Multiscale Physics-based Modeling for Dynamic Deformation and Dynamic Failure of Advanced Ceramics (Daphalapurkar, JHU)
- TEM and APT Characterization of Boron Carbide (Hemker, JHU)

Mitigation of Amorphization in Boron Carbide Through Si Doping

Mr. Anthony Etzold *Rutgers University*	**Professor Richard Haber** *Rutgers University*	**Dr. Vlad Domnich** *Rutgers University*
Dr. Atta Khan *Rutgers University*	**Dr. Kris Behler** *U.S. Army Research Laboratory*	**Dr. Jerry LaSalvia** *U.S. Army Research Laboratory*

Boron carbide is well known as an exceedingly hard material and along with its low density and exceptional resistance to wear is a prime candidate for armor materials. However, its low fracture toughness and powder issues stemming from current industrial processing techniques are detrimental for its use as a material for multi-impact armor. At Rutgers, we have enhanced the properties of boron carbide powders through Rapid Carbothermal Reduction processing which has had an immediate impact on the hardness and strength of armor plates. While these measures solve some macroscopic issues, the low fracture toughness has been addressed through modifying the crystal structure with the addition of silicon. This work has successfully incorporated silicon into boron carbide and reduced the amount of amorphization boron carbide undergoes under stress. As amorphization is a key component in the failure of boron carbide, this reduction signifies advancement in toughening the material for use in armor.

Initial work was done in conjunction with Dr. Behler at ARL, by coupling boron carbide with a boron silicide at high temperature for extended timeframes to map the diffusion of silicon into boron carbide using ARL sintering equipment. Observations of this material at varying silicon levels along the diffusion zone were done using Energy Dispersive X-ray Spectroscopy to map diffusion. Amorphization data was obtained via Raman by observing the material before and after indentation. The analysis of silicon doped boron carbide showed as much as a 60% reduction in the intensity of amorphous peaks in Raman when compared with those of standard boron carbide validating the initial concept. Using the stoichiometry obtained from the diffusion zones, bulk material synthesis was possible allowing for the use of X-ray diffraction. Rietveld refinement of these patterns in conjunction with electron density Fourier maps show the silicon atoms within the boron carbide lattice replacing the central boron atom of the three-atomic chain to result in a C-Si-C kinked chain. By adopting this formation, the silicon atom lies close to the icosahedra and seems

to have bonding with the nearest boron atom of the icosahedra, possibly further stabilizing it. This additional stabilization may have led to the observed reduced amorphization. Currently, we are awaiting TEM results from Dr. Kelvin Xie of JHU to obtain visual evidence of the reduced amorphous zones beneath the indents to verify the Raman results.

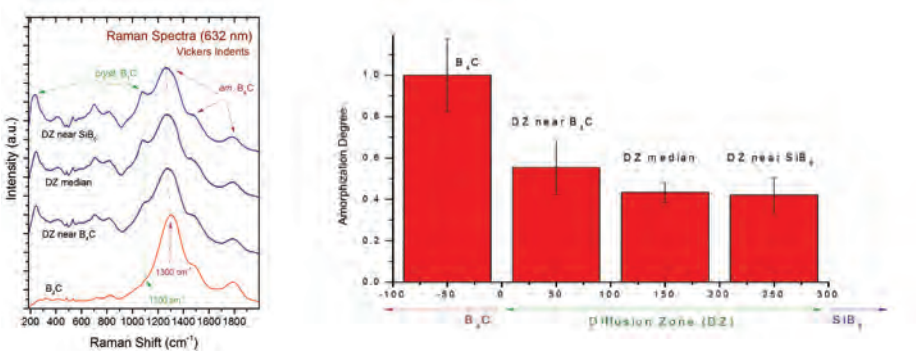


Figure 6: *Raman analysis of indented samples and graph depicting reduction of amorphization.*

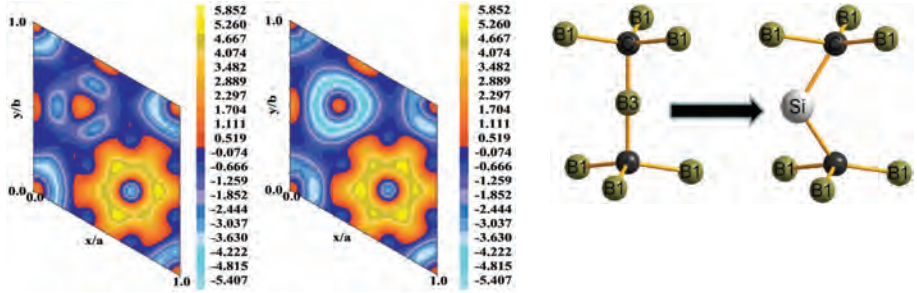


Figure 7: *Electron Density Maps based on XRD refinement and model of new chain structure.*

In Situ Visualization of Fracture in Boron Carbide

Dr. Andrew Leong
Johns Hopkins University

Professor Todd Hufnagel
Johns Hopkins University

Dr. Daniel Casem
U.S. Army Research Laboratory

Dr. Brian Schuster
U.S. Army Research Laboratory

Dr. Chris Meredith
U.S. Army Research Laboratory

Professor K.T. Ramesh
Johns Hopkins University

Dr. Nicholas Sinclair
Washington State University

In the development of armor ceramics, boron carbide is an attractive material because it is lightweight with high hardness and wear resistance. However, processing of boron carbide to high densities can produce unwanted defects and inhomogeneities that become sites for crack nucleation. A detailed understanding of the behavior of these cracks becomes important in characterizing boron carbide for use in military and industrial related applications. But common experimental methods provide only limited information about the behavior of cracks — for example, examining the fracture surface after the fact, or using optical imaging to see the advance of the crack on the sample surface.

Using synchrotron x-ray microcomputed tomography, researchers from JHU have measured the spatial and size distributions of flaws (pores and inclusions) in samples of boron carbide (Fig. 8), which provides insight into likely sites for crack initiation. To visualize the initiation and propagation of these cracks directly, JHU and ARL researchers have collaborated to perform dynamic fracture tests in situ at the Advanced Photon Source (APS) using high-speed x-ray phase contrast imaging (XPCI). Knowing the initial microstructure and the crack dynamics, our next goal is to correlate the two data sets to understand how the defects influence the crack behavior. A related project, led by Dr. Andrew Leong, is to develop an algorithm to quantify material damage (crack number density and size distribution) and use the results of simulations based on this algorithm to calibrate and validate computational models of dynamic fracture.

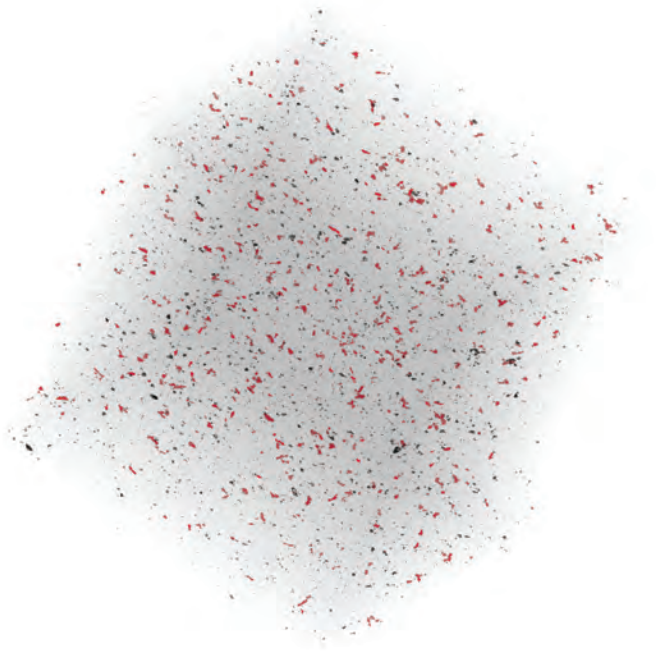


Figure 8: *3D reconstruction of boron carbide displaying spatial distribution of pores (black) and graphitic disks (red)*

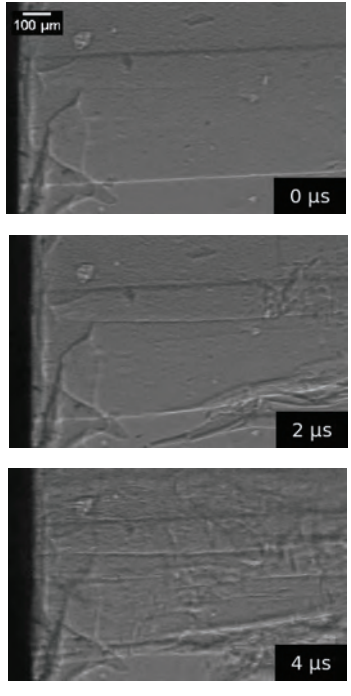


Figure 9: *A sequence of 2D phase contrast X-ray images of boron carbide undergoing uniaxial compression.*

Granular Flow in Boron Carbide

Professor K.T. Ramesh
Johns Hopkins University

Dr. Andrew Tonge
U.S. Army Research Laboratory

Mr. Xiangyu (Alex) Sun
Johns Hopkins University

Brittle materials like ceramics break easily, producing fragments. A number of applications of advanced ceramics involve largely compressive states (such as developed during impact). In such applications, in the first stage of deformation the ceramic cracks. Next, the cracks grow and eventually intersect to form fragments, and finally, the fragments deform and move with respect to each other in a kind of deformation that is called a granular flow. The properties of this granular medium under the high pressures developed during impact are very poorly understood.

We have previously developed material models that assume granular flow, but have never had good experimental data to establish the usefulness of such models. The key accomplishment here is the direct measurement of the granular flow properties of an advanced ceramic under high pressures and high strain rates. We used a pressure-shear plate impact experiment to measure the behavior of a commercial boron carbide powder over timeframes of ~ 1 microsecond, pressures of about 2 GPa, and shear strain rates of 10^5 s^{-1}. These are conditions similar to those developed under impact, or developed within the critical shearing region in some kinds of earthquakes.

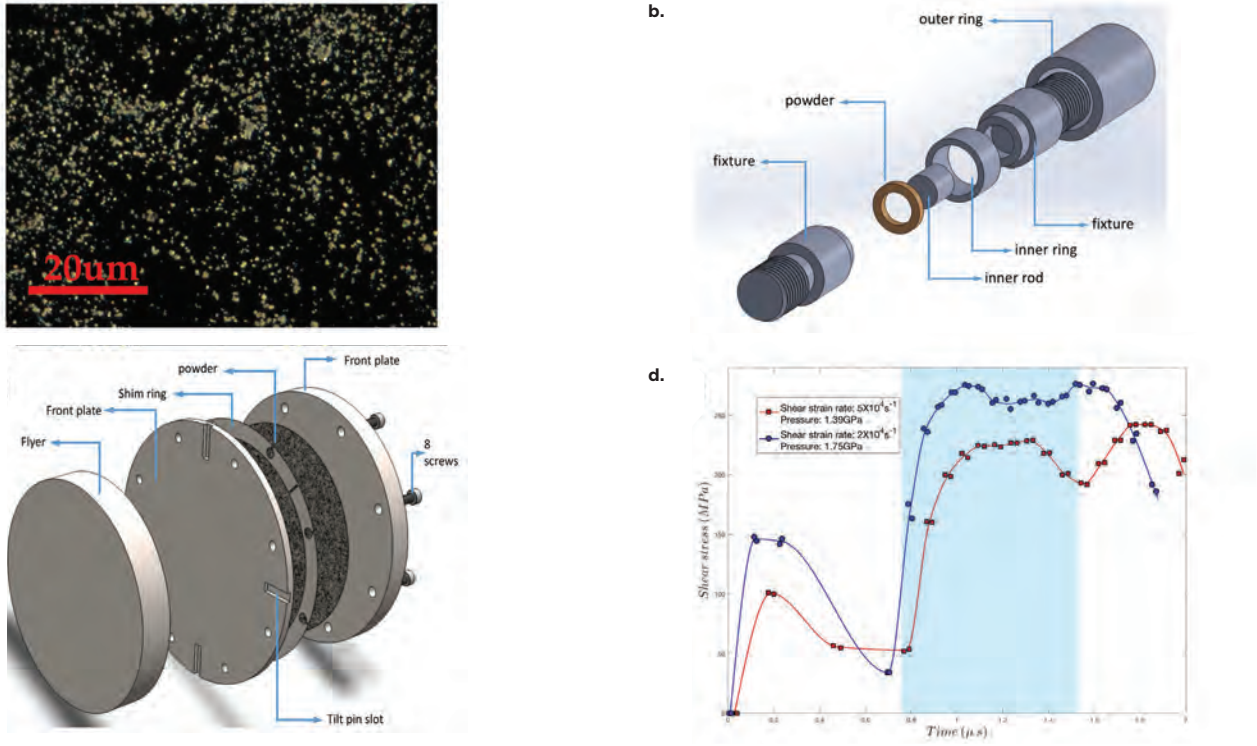


Figure 10: *(a) ESK 3000F commercial boron carbide powder; (b) Schematics for pressure shear plate impacted experiment; (c) Schematics compression torsion bar experiment; (d) Typical granular flow shear stress under two different pressure levels.*

ANTHONY ETZOLD

Ph.D. Candidate, Rutgers University

MEDE Area of Research:
Control of Inelastic Mechanisms in Boron Carbide Through Processing

> "The MEDE program has had a large impact on my research well beyond acting as my source of funding in pursuing my PhD. The chance to work with the researchers at ARL and see firsthand the end goal application some of my research will be attributed to, supplied not only deeper insight into the project but also supplied an increase in drive for the project as a means to help protect the members of our armed forces. The cooperation brought about by MEDE between the universities and ARL has helped to streamline much of the research I have been working on by processing material both at Rutgers and at ARL, utilizing equipment I would otherwise not have access to. Similarly, having members of ARL come to Rutgers to characterize their own samples allowed for close collaboration even between projects."

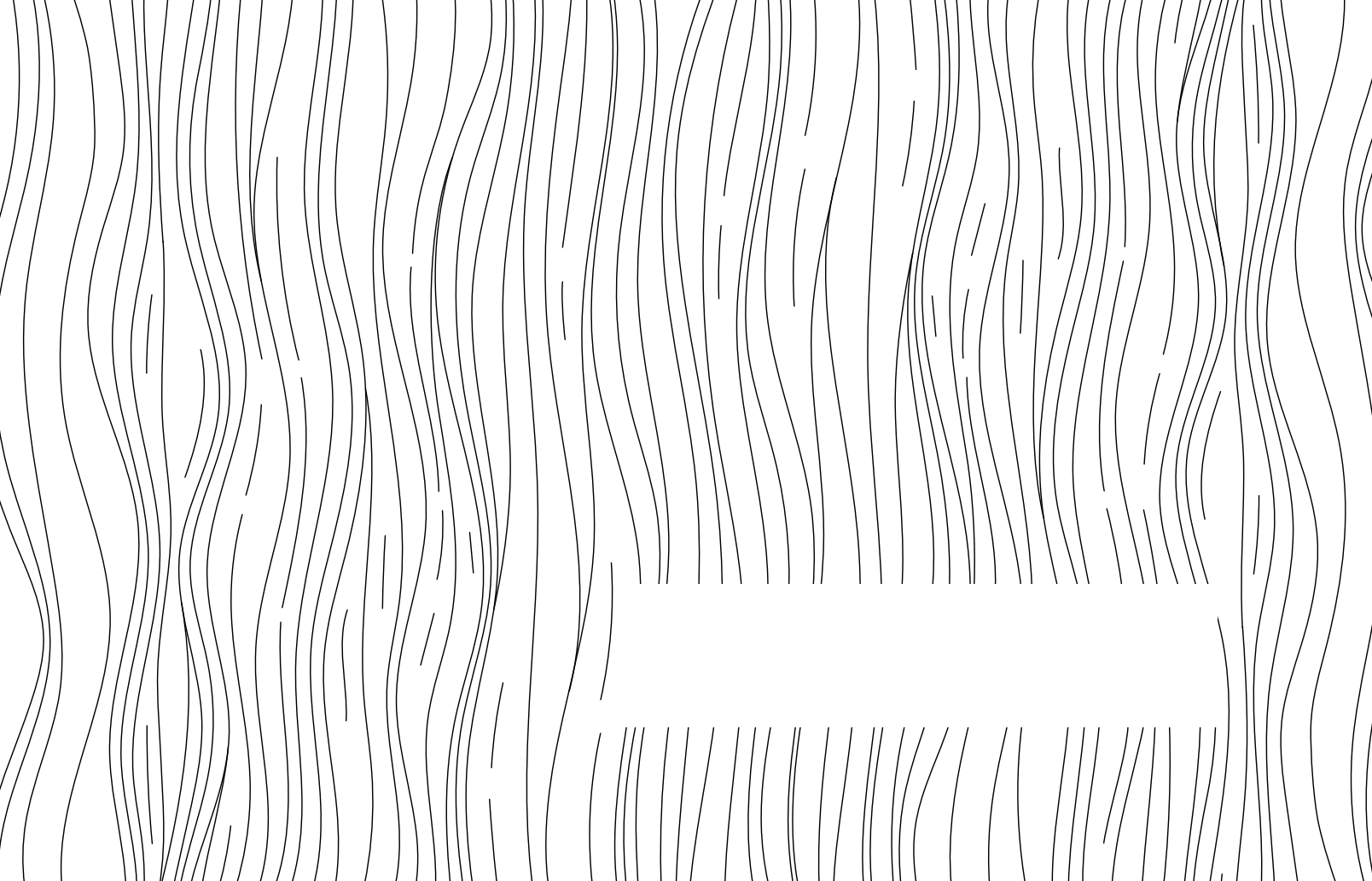
PROF. NITIN DAPHALAPURKAR

Assistant Research Professor, Department of Mechanical Engineering and Hopkins Extreme Materials Institute, Johns Hopkins University

MEDE Area of Research:
Integrated Multiscale Physics-based Modeling for Dynamic Deformation and Dynamic Failure of Advanced Ceramics

"Ceramics, watching them fail under impact is a 'thrilling' experience. Because, no two material specimens fail exactly alike. Developing a coherent understanding for brittle failure of boron carbide requires developing advanced theories of damage due to microscopic cracks, amorphization and other inelastic mechanisms. This collaborative effort towards developing advanced models and simulations, with a vast number of ARL scientists and academic colleagues, has been highly fulfilling."

Artistic rendering of a cross-section of the S-2 Glass/Epoxy composite material.



COMPOSITES

Consortium Lead - Prof. John W. Gillespie, Jr. (Delaware)

ARL Lead - Dr. Daniel J. O'Brien

Composites CMRG

CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Cameron Abrams, Drexel

Prof. Suresh Advani, Delaware

Prof. Kadir Aslan, Morgan State

Prof. Wayne Chen, Purdue

Dr. Sanjib Chowdhury, Delaware

Prof. Somnath Ghosh, JHU

Prof. John W. Gillespie, Jr., Delaware

Prof. Lori Graham-Brady, JHU

Prof. Bazle Haque, Delaware

Prof. Giuseppe Palmese, Drexel

Prof. Shridhar Yarlagadda, Delaware

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Dr. Joe Lenhart

Dr. Kevin Masser

Mr. Chris Meyer

Dr. Daniel J. O'Brien

Dr. James Sands

Dr. Timothy Sirk

Dr. Tusit Weerasooriya

Dr. Chian Fong Yen

CONSORTIUM RESEARCH TASKS

- Characterization of Composite Materials (Aslan, Morgan State)
- Epoxy Molecular Simulations (Abrams and Palmese, Drexel)
- Meso-Mechanical Modeling of Canonical Perforation Experiments (Haque and Gillespie, Delaware)
- Micromechanical FE Modeling of Tensile Failure of Unidirectional Composites (Gillespie, Delaware)
- Micro-Mechanical Modeling of Progressive Punch-Shear Behavior of Uni-Directional Composites (Gillespie and Haque, Delaware)
- Multi-scale Modeling of Damage and Failure in Composites (Ghosh, JHU)
- Multi-scale Modeling of Fiber-Matrix Interphase (Gillespie and Chowdhury, Delaware)
- Real-time Damage Visualization in Polymers and Composites (Chen, Purdue)
- Synthesis and Characterization of Interphases and Tows with Controlled Resin Distribution (Advani and Yarlagadda, Delaware)
- Synthesis of Epoxy Networks and Interphases with Controlled Topology (Palmese and Abrams, Drexel)

Multi-Scale Modeling of Fiber-Matrix Interphase

Dr. Sanjib C. Chowdhury	Professor John W. Gillespie, Jr.	Dr. Robert M. Elder	Dr. Timothy W. Sirk
University of Delaware	*University of Delaware*	*U. S. Army Research Laboratory*	*U. S. Army Research Laboratory*

In glass fiber epoxy composites, interphase is a distinct region between fiber and epoxy matrix which controls composite properties by controlling load transfer and failure modes. Interphase develops during processing through diffusion and reaction between the matrix and the fiber sizing. It is a complex mixture of sizing (silane, film former and surfactant), curing agent and epoxy matrix. Interphase thickness in glass-epoxy composites varies from 10-100nm and its properties depend on its structure and its interaction with glass surface and epoxy resins. The complex formation mechanism and morphology of the interphase at the nano-meter length-scale is still not well understood. To design optimum interphase with higher strength and toughness, it is imperative to have complete understanding of the interphase process-structure-properties relationship.

In this research, we are establishing a materials-by-design framework for glass-epoxy composite interphases using molecular dynamics (MD) simulations. This framework includes optimizing structure of individual constituents – glass, sizing and epoxy and optimizing inter-constituent interaction. Recently, we have studied the structure-properties relationship of sizing [1] and interaction of silane, which is major a component in sizing, with glass surface [2]. We found that sizing properties could be tailored by changing the network composition and structure which could be achieved by changing process conditions. Sizing structure with higher percentage of T3 species gives high stiffness, strength (3-4 times the epoxy properties) and toughness, while sizing structure with higher percentage of T2 species gives low stiffness and strength but have the highest elongation. Similarly, glass-sizing interphase strength and energy absorption capability could be tailored by changing the silane bond density with the glass surface. Mixed mode traction-separation law for interphase is developed from MD predictions and it will be used to bridge length scales in finite element analysis for fracture modeling of the fiber-matrix interphase having different thickness in composites subjected to mixed-mode loading. Overall, this MD framework will enable us to understand the interphase chemistry, interphase formation mechanism, deformation and damage mechanics and properties tailoring mechanism.

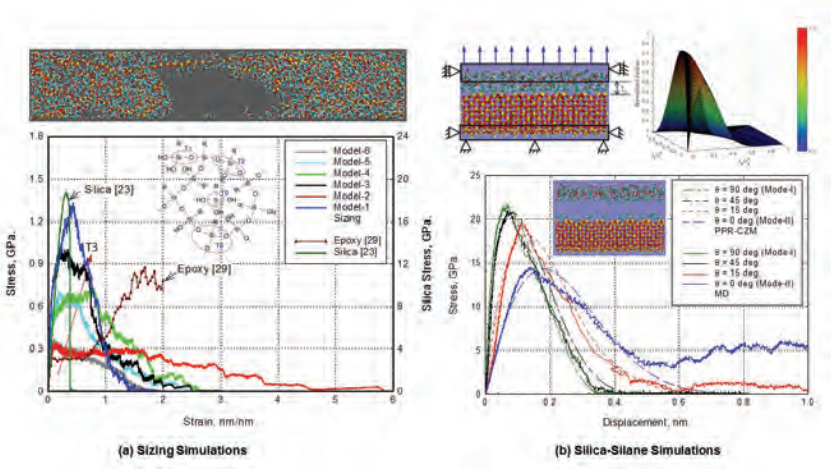


Figure 11: *(a) Stress-strain response of sizing layer with various morphology, and (b) Mixed-mode traction-separation response of silica-silica interphase. (Corresponding failure modes are also shown.)*

References:

1. Chowdhury S. C., Elder R. M., Sirk T. W., Adri C. T. van Duin, and J. W. Gillespie, Jr., "Modeling of glycidoxypropyltrimethoxy silane compositions using molecular dynamics simulations", Computational Materials Science, 2017, 140: 82-88..

2. Chowdhury, S. C., and J. W. Gillespie, Jr., "Silica - silane coupling agent interphase properties using molecular dynamics simulations," Journal of Materials Science, 2017, 52: 12981-12998.

3. Chowdhury, S. C., B. Z. (Gama) Haque, J. W. Gillespie, Jr., "Molecular Dynamics Simulations of the Structure and Mechanical Properties of Silica Glass using ReaxFF", Journal of Materials Science, 51 (22), pp. 10139-10159, 2016.

Micromechanical Finite Element Modeling of Tensile Failure of Unidirectional Composites

Professor John W. Gillespie, Jr.
University of Delaware

Dr. Daniel J. O'Brien
U.S. Army Research Laboratory

Mr. Raja Ganesh
University of Delaware

Unidirectional tensile strength is one of the most important properties governing the dynamic performance of composite materials. State-of-the-art micromechanics models consider failure as a quasi-static process. In our study, the evolution and localization of micromechanical damage in S Glass/Epoxy is found to be a highly dynamic process [1] (local strain rates are predicted to be on the order of 10^5-10^6 /s). This process involves a sequence of interrelated damage mechanisms: i) brittle fiber breaks (which depend on the statistical distribution of critical defects within the fiber [2]), ii) propagation of dynamic stress concentrations as tensile stress waves over large distances in the fibers adjacent to the fiber break, iii) localized plastic yielding of the matrix due to high shear strains and iv) dynamic debond propagation in the interface surrounding the broken fiber (Figure 12a). Since the stress waves in the fibers travel at the sound speed in S2-glass (6 km/s), the time-scales associated with these dynamic mechanisms are of the order of 1-100 nanoseconds [3] and the length scales of interest are 1-1000 microns. The overall goal of this project is to create a detailed Finite Element (FE) modeling framework to predict the evolution of these dynamic micro-mechanical damage mechanisms and their interactions as a function of the constituent properties of the fiber, matrix and interphase.

The results indicate that the dynamic stress redistribution around a fiber break is heavily influenced by the amount of energy dissipated through interfacial debonding and matrix plasticity [4]. The ratio of shear yield strength in the matrix to the mode II peak traction in the interface, R_{shear}, is identified as an important material parameter controlling the transition in damage modes from purely matrix yielding to a combination of matrix yielding and interfacial debonding. A criterion for unstable debonding of the interface (Figure 12b), which can lead to axial splitting failure mode of the composite [5], has been established as a function of the energy absorption capacity of the interface traction laws. Our results show that an optimal combination of constituent properties are required to improve unidirectional tensile properties of the composite.

The modeling framework serves as an integrative model of lower length-scale constitutive models for the fiber, matrix and interphase and provides valuable feedback to our collaborators at MEDE in terms of tailoring the matrix and interphase as a system to maximize strength and overall energy absorption in unidirectional composites. Additionally, this modeling effort will also provide inputs to homogenized composite continuum damage models at higher length-scales

References:

1. Ganesh R, Sockalingam S, (Gama) Haque BZ, Gillespie Jr. JW, "Dynamic effects of single fiber break in unidirectional glass fiber-reinforced composites", Journal of Composite Materials 2017;51:1307–20.

2. Ganesh R, Loesch R, Henderson E, Gillespie Jr. JW, "Experimental determination of strength distribution of S2-glass fibers across a wide range of gage lengths", Proceedings of the American Society for Composites - 32nd Technical Conference, West Lafayette, IN, 2017.

3. Ganesh R, Sockalingam S, Gama Haque BZ, Gillespie JW, "A finite element study of dynamic stress concentrations due to a single fiber break in a unidirectional composite", Proceedings of the American Society for Composites - 31st Technical Conference, Williamsburg, VA, 2016.

4. Ganesh R, Sockalingam S, and Gillespie Jr. JW, "Dynamic effects of single fiber break in unidirectional glass fiber-reinforced composites: Effects of matrix plasticity", Journal of Composite Materials, 2017. DOI: 10.1177/0021998317737604.

5. Shokrieh MM, Omidi MJ, "Tension behavior of unidirectional glass/epoxy composites under different strain rates", Composite Structures 2009;88:595–601.

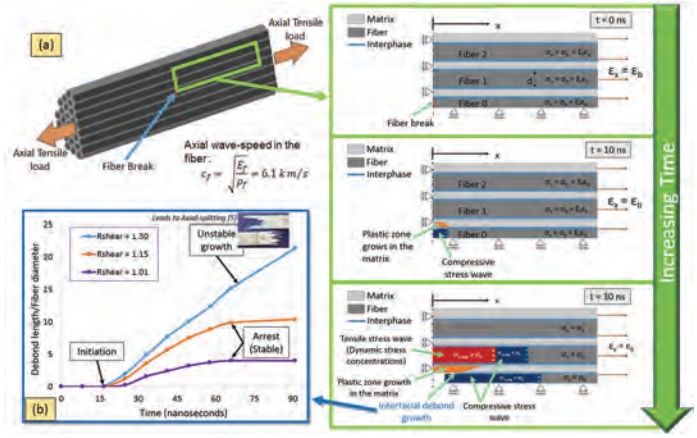


Figure 12: *(a) Dynamic progression of events after a fiber break (b) Transition from stable to unstable interfacial debonding with increasing* R_{shear}.

MR. ENOCK BONYI

Doctoral Student, Morgan State University

MEDE Area of Research:
Assessment and Quantification of Ballistic Damage of a Single Layer Woven Fabric Composite Laminate

> "The opportunity to participate in the MEDE program has and continues to expand my knowledge and widen my experiences in material science especially in damage characterization and quantification. The insights, ideas, and contributions — especially from CMRG group members from the University of Delaware and the Army Research Laboratory, are fulfilling."

DR. BAZLE Z. (GAMA) HAQUE

Senior Scientist, Center for Composite Materials, and Assistant Professor of Mechanical Engineering, University of Delaware

MEDE Areas of Research:

ARL-MSU-UD Collaborative Projects: (i) Meso-Mechanical Modeling of Canonical Perforation Experiments (ARL and UD), and (ii) Characterization of Composite Materials (MSU)

"I'm pleased to be a part of the research conducted within the Composites CMRG that showcases strong collaborative efforts. UD Professors work with ARL Scientists to develop the experimental methodology that is then used in canonical experiments at ARL. Additionally, ballistic impact damages have been characterized both at MSU & at UD, and an ARL scientist is performing multi-scale modeling of perforation experiment at UD. Through this collaboration, we've identified unique ballistic damage mechanisms and developed meso-mechanical models for fundamental understanding of perforation damage mechanics of composites."

DR. DANIEL J. O'BRIEN

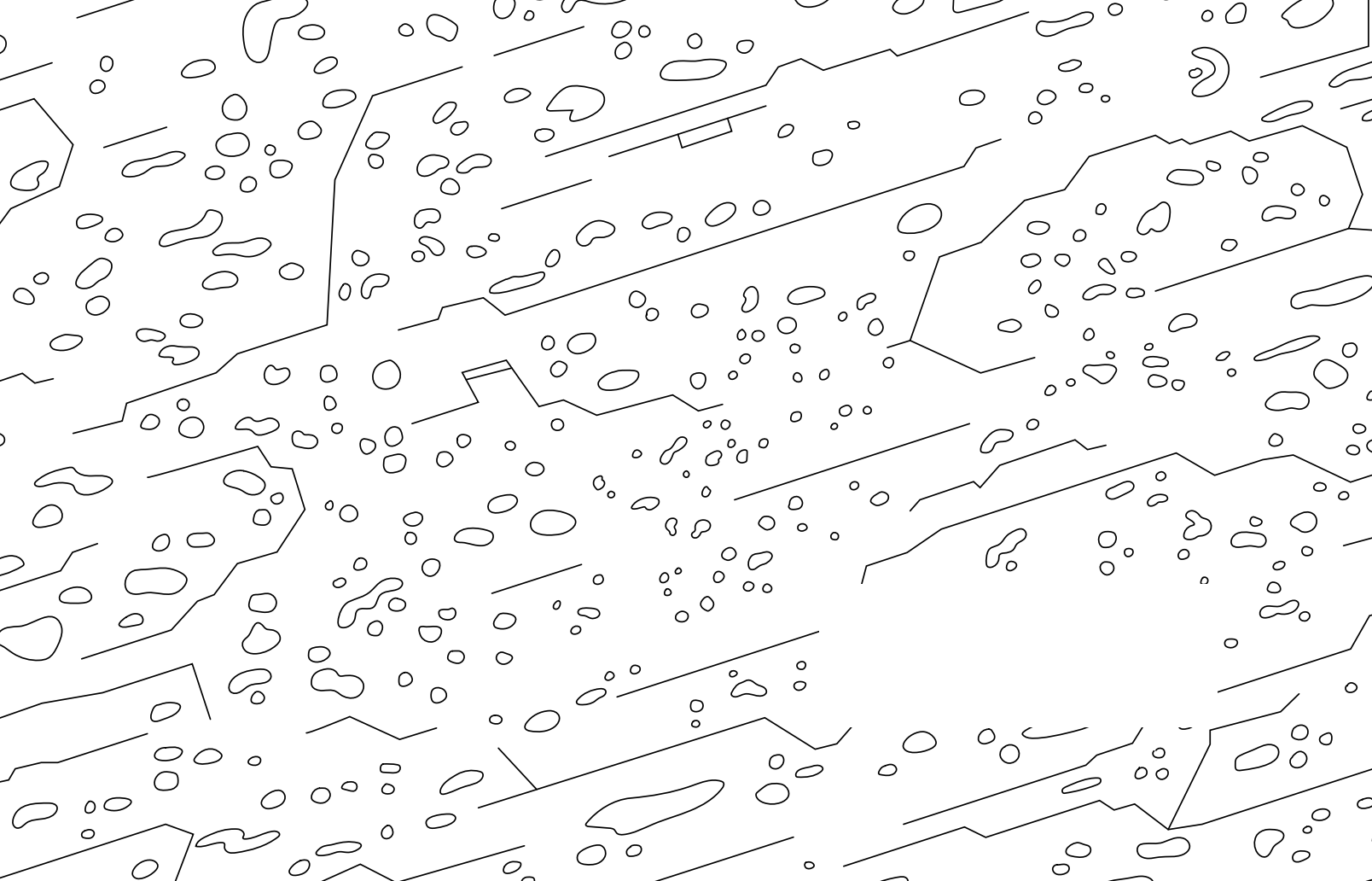
Mechanical Engineer, U.S. Army Research Laboratory

MEDE Areas of Research:

Composite Canonical Model; Multi-scale Modeling of Damage and Failure in Composites; Real-time Damage Visualization in Polymers and Composites

"In general, my work involves developing new composite materials to benefit the soldier. Through the MEDE program, we investigate the fundamental mechanisms driving composite materials performance in protection applications. MEDE has afforded me the opportunity to collaborate with talented researchers from wide-ranging disciplines to develop tools for the design of next generation armor solutions."

Artistic rendering of magnesium as seen through a transmission electron microscope.



METALS

Consortium Lead - Prof. Tim Weihs (JHU)

ARL Lead - Dr. Laszlo Kecskes

Metals CMRG

CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Kaushik Bhattacharya, Caltech

Prof. Jaafar El-Awady, JHU

Prof. Todd Hufnagel, JHU

Prof. Jamie Kimberley, NMT

Prof. Dennis Kochmann, Caltech

Prof. Michael Ortiz, Caltech

Prof. K.T. Ramesh, JHU

Prof. Jagannathan Sankar, NC A&T

Prof. Qiuming Wei, UNCC

Prof. Tim Weihs, JHU

Prof. Justin Wilkerson, UTSA

Dr. Zhigang Xu, NC A&T

Dr. Sergey Yarmolenko, NC A&T

ARL COLLABORATORS

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Dr. Todd Bjerke

Mr. Brady Butler

Dr. Daniel Casem

Dr. John Clayton

Dr. Robert Elder

Dr. Vince Hammond

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Mr. Tyrone Jones

Dr. Laszlo Kecskes

Dr. Krista Limmer

Dr. Jeffery Lloyd

Dr. Christopher Meredith

Dr. Tomoko Sano

Dr. Scott Schoenfeld

Dr. Brian Schuster

Dr. Mark Tschopp

Dr. N. Scott Weingarten

Dr. Cyril Williams

CONSORTIUM RESEARCH GROUPS

- Defects Properties Within a Grain (Bhattacharya and Oritz, Caltech; El-Awady and Weihs, JHU)
- Plasticity Across Multiple Grains (Hufnagel, Ramesh and Weihs, JHU; Bhattacharya, Caltech; Kimberley, NMT)
- Thermal Mechanical Processing (Weihs and Hufnagel, JHU; Bhattacharya and Kochmann, Caltech; Sankar and Xu, NC A&T; Wei, UNCC)
- Void Dominated Failure (Ortiz and Bhattacharya, Caltech; Wilkerson, UTSA; Weihs, JHU)

Proliferation of Twinning in HCP Metals: Application to Magnesium

Dr. Dingyi Sun
Brown University

Professor Mauricio Ponga
University of British Columbia

Professor Kaushik Bhattacharya
California Institute of Technology

Professor Michael Ortiz
California Institute of Technology

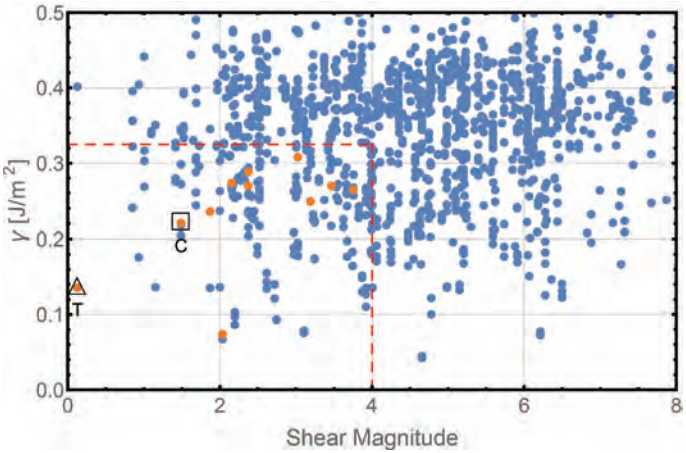
Twinning — the reorientation of a material's lattice about a plane of discontinuity — is one of the prominent mechanisms by which materials can accommodate deformation. Present in a wide variety of different materials, twinning appears most prolifically in hexagonal close-packed (HCP) metals, such as magnesium (Mg), where it is one of the favored mechanisms by which out-of-plane deformations are accommodated. Although two particular modes of twinning — the compression and tension twins — have been widely accepted in the community, multiple observations of additional, so-called "anomalous" modes have occurred over the years.

In order to address the existence of these "anomalous" modes and also explore whether or not additional modes are plausible and relevant during deformation, we developed a systematic framework which drew on information from a variety of length scales to provide insight on the matter. We began by kinematically predicting a vast set of potential twin modes. We then assessed the energetics of these twins using atomistic simulations. The information ascertained from atomistics was then used to synthesize a yield surface for the material that took into account all of these newly-predicted modes of twinning and returned the modes which were likely to be observed under deformation.

Applying this framework to magnesium, we found that the twinning landscape is drastically more diverse than what has been previously acknowledged. Over the course of our investigation, we found that there were multiple twin modes that were predicted to affect yield behavior in magnesium; some of these modes, although irrational, were very close in configuration to previously observed modes that had been labeled "anomalous." This discovery has motivated us to extend the work to the investigation of alloys, where we will be using this framework to investigate how new twin modes may be exploited for the design of a new generation of improved magnesium alloys and alloys based on other HCP metals.

Figure 13: *(a) Scatterplot of twin interface energy against shear magnitude; red dashed line shows region of interest incorporating previously-observed twin modes, and orange points represent modes which are predicted to affect yielding in magnesium, including the tension (T) and compression (C) twin modes. (b) Representative slices of the magnesium yield surface, showing a slice with bunching of twin modes near the magnesium yield surface, and a slice where the yield surface is governed by multiple, non-classical twin modes.*

a.



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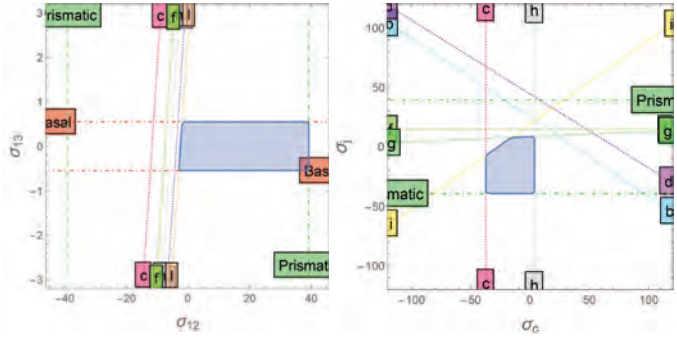


Understanding the Microstructural Evolution of Mg Through In-situ Neutron Diffraction

Mr. Nicholas M. Krywopusk
Johns Hopkins University

Dr. Laszlo J. Kecskes
U.S. Army Research Laboratory

Dr. Matthew J. Frost
Oak Ridge National Laboratory

Dr. Alexandru D. Stoica
Oak Ridge National Laboratory

Professor Todd C. Hufnagel
Johns Hopkins University

Dr. Ke An
Oak Ridge National Laboratory

Professor Timothy P. Weihs
Johns Hopkins University

Equal Channel Angular Extrusion (ECAE) of magnesium has proven effective in grain size refinement and texture modification. This microstructural evolution is due to the process of dynamic recrystallization (DRX). Multiple mechanisms of DRX in magnesium are possible, and are generally categorized into continuous and discontinuous behavior. Different mechanisms of DRX can produce different microstructures and textures. However, understanding DRX and its controlling mechanisms has proven difficult to achieve using ex-situ experiments. To remedy this gap in our understanding, we designed and constructed a heating and backpressure capable ECAE die that was used to extrude highly textured pure magnesium at the VULCAN beamline at SNS. Three temperatures and two texture orientations were interrogated using the neutron transparent ECAE die.

While the overall objective is to better understand how to control DRX mechanisms, the experiment sought to use peak profile evolution to accomplish three specific objectives: the size of the recrystallized nuclei, the temperature dependence of the onset of recrystallization and final grain size, and identification of the active DRX mechanisms. Each of these objectives was selected for the importance it has in designing and improving magnesium extrusion routes.

Analysis of the collected data is ongoing, but some initial results are available. Magnesium extruded in both orientations was observed to undergo a significant amount of twinning shortly after the extrusion began. The result is that both orientations rapidly acquire a texture suited for basal slip. Ex-situ Electron Backscatter Diffraction (EBSD) of the samples confirms that a significant area fraction of the material is recrystallized, and the resulting texture is complex, suggesting that both basal slip and prismatic slip are active during deformation and recrystallization.

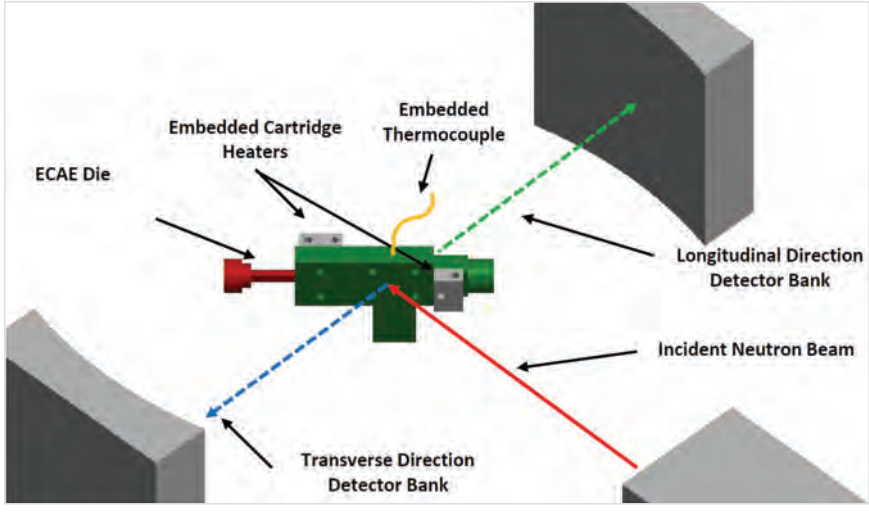


Figure 14: *Schematic of the neutron diffraction experiment. The backpressure system is not included. Diffraction data was collected simultaneously from both the transverse and longitudinal directions.*

MR. VIGNESH KANNAN

Graduate student, Johns Hopkins University

MEDE Area of Research:
High Strain Rate and High Temperature Characterization and Shear Localization of Mg and Its Alloys

> "I came into the MEDE program as a naive, uninitiated graduate student, but the strong interdisciplinary environment has made my journey in academic research a joyful and exciting one. The opportunity to be able to interact and learn from a team of experts looking at different pieces of a complex problem, on a regular basis has been a continuous source of inspiration; an integral part in my grooming as researcher."

PROF. JAMIE KIMBERLEY

Associate Professor, New Mexico Institute of Mining and Technology

MEDE Area of Research:

Plasticity Across Multiple Grains

"The MEDE program has provided ample opportunity to collaborate with researchers on the forefront of materials research. These collaborations are critical to the success of the program, and have allowed the consortium to make significant progress toward a multi-scale, mechanism-based, materials design methodology. Furthermore, working closely with this diverse set of researchers has allowed me to develop a new perspective on how my expertise can improve our understanding of material response at the extremes."

DR. JEFF LLOYD

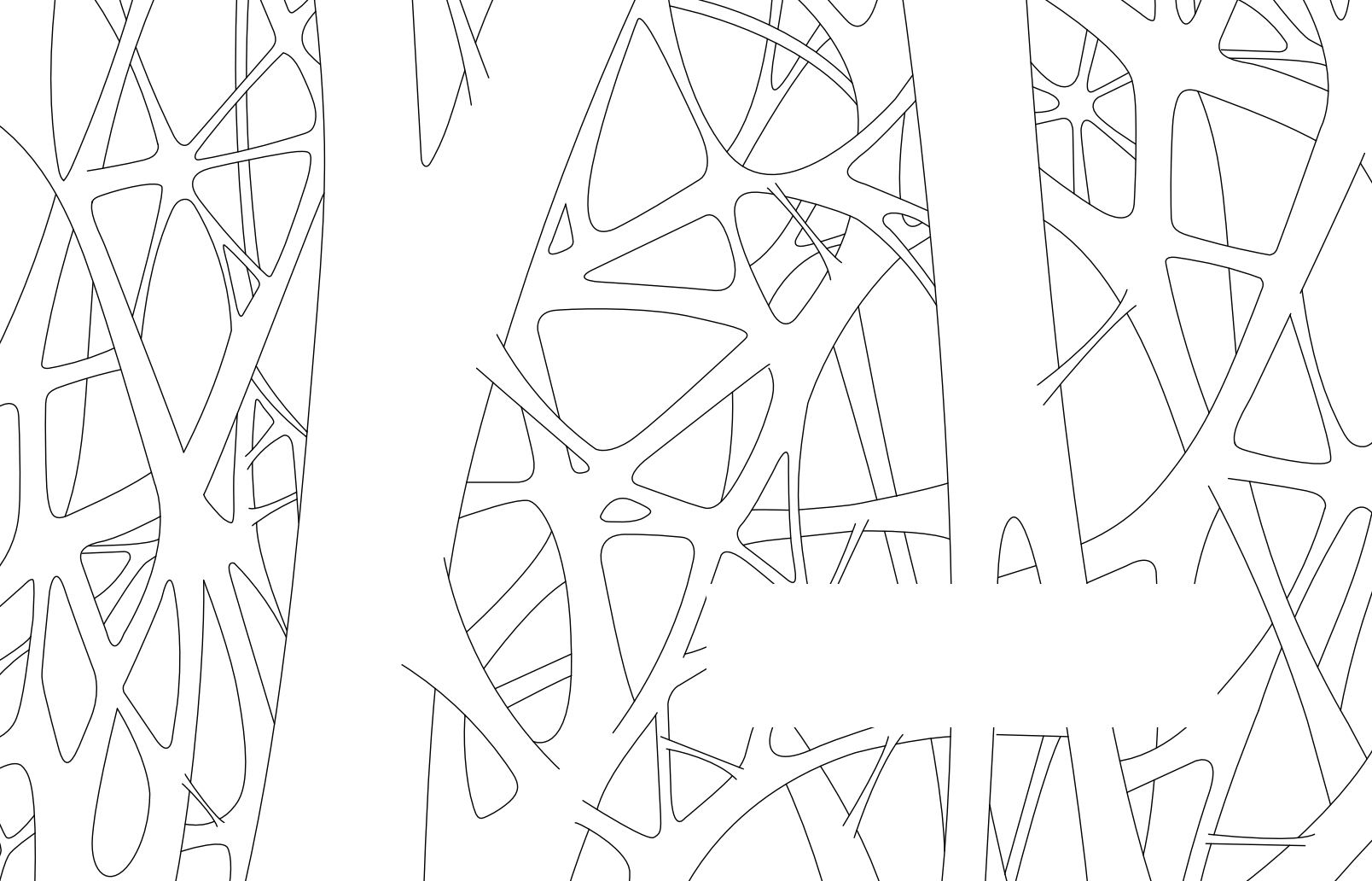
Research Scientist, U.S. Army Research Laboratory

MEDE Areas of Research:

Modeling Plasticity Within a Grain, Across Grains; Void Dominated Failure

"Learning about magnesium within MEDE has been challenging but rewarding — it is lower symmetry than most conventional metals, very light, deforms quite differently when loaded in different directions, and when you mention you work on it all people want to talk about is lighting it on fire in their high school chemistry class. The best thing though, is that once you understand how magnesium behaves, understanding the behavior of aluminum, titanium, copper, and other metals is really easy. The opposite is not true."

Artist rendering of polyethylene fiber as seen through an atomic force microscope.



POLYMERS

Consortium Lead - Prof. Giuseppe Palmese (Drexel)

ARL Lead - Dr. James Snyder

Polymers CMRG

CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Nicolas Alvarez, Drexel

Dr. Joseph Deitzel, Delaware

Prof. John W. Gillespie, Jr., Delaware

Prof. Vicky Nguyen, JHU

Prof. Giuseppe Palmese, Drexel

Prof. Mark Robbins, JHU

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Dr. Jan Andzelm

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Dr. Kevin Masser

Dr. Kenneth Strawhecker

Dr. James Snyder

Dr. Tusit Weerasooriya

CONSORTIUM RESEARCH TASKS

- Fabrication and Processing (Alvarez and Palmese, Drexel; Deitzel and Gillespie, Delaware)
- Mapping Defects and Linking Failure Modes at Multiple Length Scales in UHMWPE Filaments (Deizel and Gillespie, Delaware)
- Micromechanical Model for the Strength and Failure Behavior (Nguyen, JHU)
- Modeling and Experiments of High Performance Polymer Fibers Subjected to Transverse Compression Loading (Gillespie, Delaware)
- Modeling Polymer Deformation: Potentials and Methods (Robbins, JHU)

Correlations between Fiber Morphology and Tensile Properties in UHMPE Fiber Production

Professor Nicolas Alvarez	**Professor Giuseppe Palmese**	**Dr. Joseph Deitzel**	**Dr. Ken Strawhecker**
Drexel University	*Drexel University*	*University of Delaware*	*U.S. Army Research Laboratory*

Gel-Spun UHMWPE (ultra-high molecular weight polyethylene) fibers fill a need for lightweight, strong durable materials in Army personnel and vehicle protection. MEDE collaborators at JHU have recently shown that the theoretical limit for UHMWPE fibers composed of finite chain lengths is a strength of ~7 GPa. While fiber strengths ranging from three to seven GPa have been reported in the literature, we lack a fundamental correlation between fiber morphology (crystalline microstructure) and bulk tensile strength. Using two novel apparatuses designed and built by Drexel researchers for the MEDE project, we can examine the evolution of UHMWPE fiber morphology throughout the entire processes of gel spinning and fiber drawing.

Utilizing the unique features of our gel-spinning device, we have determined the effects of strain, strain rate and nozzle design on crystalline structure formation during gel-spinning. For example, fibers spun under increasing strain rates, exhibit increasing crystallization rates. This phenomenon is known as extensional flow-induced crystallization (FIC) kinetics and is not well understood. Drexel has shown that the Weissenberg number (Wi=$\dot{\epsilon}\tau_d$), a measure of propensity for chain stretching, captures the transition from isotropic lamellae to stretched crystal transition in the final spun fiber, see Figure 15. In other words, a final fiber structure during spinning is solely determined by the Wi and the amount of strain before crystallization. Using a novel drawing apparatus, the As-Spun fibers are then drawn under highly controlled conditions to understand the evolution of structure as a function of strain, stretch rate, and temperature. This apparatus also allows for in-situ measurements of fiber tensile properties at any time during drawing. The result is fiber samples with well described processing history, offering a unique opportunity to understand morphology evolution during the fiber production process. These unique fiber samples are distributed to collaborators within the MEDE program.

The As-Spun and Drawn fibers are examined using thermal analysis to determine crystalline fractions at UD-CCM, SAXS and WAXS to determine crystalline structure and morphology at Drexel, and using a FIB-notch AFM technique to image the inter-fiber structure at ARL. The goal of these studies is to make key correlations between processing/fiber morphology and ultimately

fiber morphology/tensile properties. One interesting result at present is that there appears no correlation between the crystalline structure as probed by SAXS (10-100 nm length scales) and tensile modulus for a given fiber. The corresponding Figure shows tensile modulus data for very different crystalline morphologies as seen from the SAXS 2D scattering patterns (insets). Instead of showing unique relationships for modulus and draw ratio for a given crystalline morphology, the figure shows that all crystalline structures show the same modulus as a function of draw ratio. Examining only SAXS patterns is not enough to make a correlation between structure and tensile properties. However, using the combination of the different analytical techniques outlined above, we expect to formulate a clear picture between structure and mechanical properties.

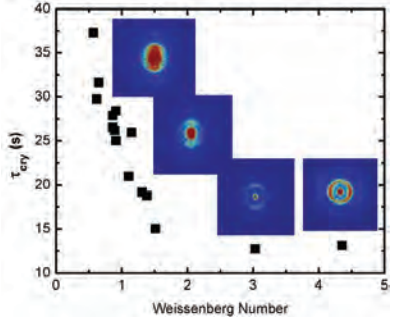


Figure 15: *Crystallization time (s) as a function of the applied Weissenberg Number. Crystallization time decreases as Wi increases up to a Wi of 1.5, after which the time stops decreasing further. 2D SAXS patterns are shown for select points on the curve. We observe a transition from a polydisperse lamellar structure at the low Wi transitions to a highly ordered structure at high Wi number.*

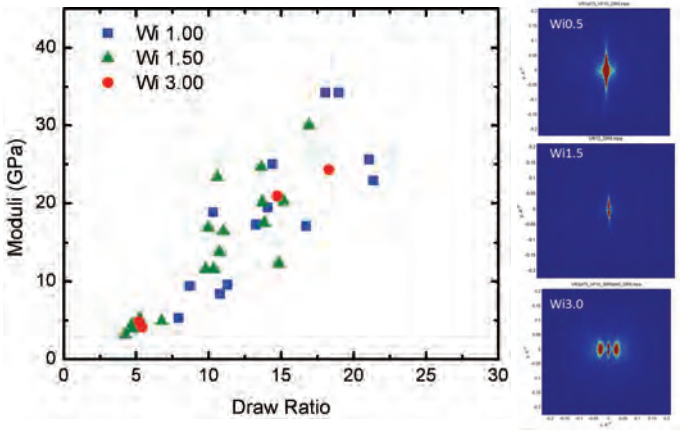


Figure 16: *Tensile modulus versus draw ratio for three as-spun fibers generated from different Wi numbers. All three fiber morphologies (although very different) lead to the same modulus versus draw ratio trend. The insets show how different the structures are at DR=10 via 2D SAXS patterns.*

MR. CHRISTOPHER HENRY

Ph.D. Candidate, Drexel University

MEDE Area of Research:
Synthesis of UHMWPE Fibers

> "I work full-time on materials relating to the MEDE project. The collaborators that I have had a chance to work with through the program have not only broadened my approach to research, but have deepened my understanding in my field. I am immensely grateful to the MEDE program for the opportunities it has given me."

PROF. NICOLAS ALVAREZ

Assistant Professor, Drexel University

MEDE Area of Research:
Polymer Processing

"Our focus in the MEDE program is to make quantitative connections between processing history and material tensile properties, as they relate to ultra-high MW Polyethylene (UHMWPE). UHMWPE has shown great promise as a material in extreme environments, e.g. ballistic armor, without a fundamental understanding of why. Some may be surprised to know that our processing effort was not part of the initial polymer CMRG tasks. If not for the prudence of the MEDE governing board, our team's involvement and scientific achievements within the program would be absent. I owe many thanks to the board and our CMRG colleagues for the many discussions and interactions that have led to unparalleled advancements in the field."

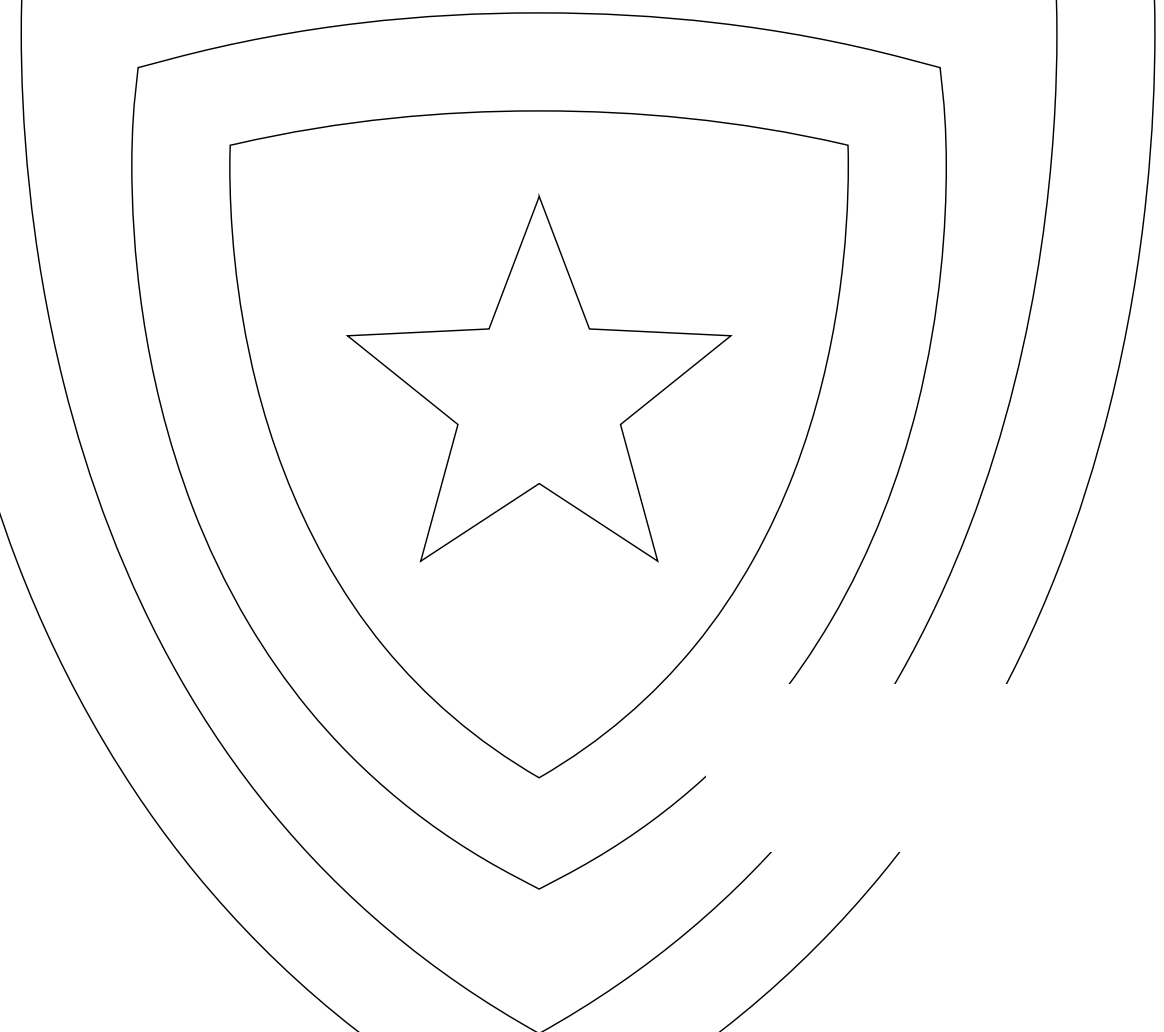
DR. TRAVIS A. BOGETTI

Mechanical Engineer, Composites and Hybrid Materials Branch, Materials and Manufacturing Science Division, WMRD, ARL

MEDE Area of Research:
Polyethylene Fiber Modeling

"Polyethylene (PE) fibers possess a complex multi-scale morphology that governs their attractive ballistic response. The MEDE program has contributed significantly towards the development of physics based computational models that accurately capture the unique microstructure and associated deformation mechanics of fibrillation in PE fibers. New sub-fiber characterization techniques and data for PE fibers along with new molecular dynamics modeling potentials are helping ARL to build predictive tools that are critically needed to advance fiber performance through systematic materials-by-design studies."

The CMEDE shield symbolizes the protection and the strong collaboration found within the MEDE program.



INTEGRATIVE AND COLLABORATIVE TOOLS


Prof. K.T. Ramesh


Prof. Lori Graham-Brady


Prof. Michael Shields


Prof. Michael Kirby


Prof. Tamás Budavári


Dr. Betsy Rice


Prof. Tim Weihs


Dr. Richard Becker

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Prof. Tamás Budavári, JHU

Prof. Lori Graham-Brady, JHU

Prof. Michael Kirby, University of Utah

Prof. K.T. Ramesh, JHU

Prof. Erica Schoenberger, JHU

Prof. Michael Shields, JHU

Prof. Timothy Weihs, JHU

SELECT ARL COLLABORATORS

Dr. Richard Becker

Dr. Travis Bogetti

Mr. Brian Leavy

Dr. William Mattson

Dr. Daniel J. O'Brien

Dr. Betsy Rice

Mr. Wayne Ziegler

INTEGRATIVE RESEARCH ACTIVITIES

- Probabilistic Modeling & UQ for Computational Models of Composites (Graham-Brady and Shields, JHU)
- Data Science: Integration (Budavari, JHU)
- Development of Laser Shock Capabilities for Dynamic Materials Characterization (Ramesh, JHU)
- Novel DTEM Project (Weihs, JHU)
- Collaboration Study (Schoenberger, JHU)

Probabilistic Modeling and Uncertainty Quantification for Computational Models of Composites

Professor Lori Graham-Brady	Professor Michael Shields	Professor Michael Kirby	Professor Yanyan He
Johns Hopkins University	*Johns Hopkins University*	*University of Utah*	*New Mexico Institute of Mining and Technology*

Goal: The long-term goal of this project is to develop an efficient sampling-based framework for performing uncertainty quantification (UQ) and/or probabilistic modeling of materials in armor applications.

Research strategy: This joint team from the MEDE and MSME CRAs addresses probabilistic modeling and UQ for multi-scale models that connect lower-scale mechanisms to larger scale properties and performance. The efficient sampling framework has been applied to better understand variability in the effective behavior of composite materials and to generate free energy potentials in polymers with a small number of sample molecular dynamics simulations.

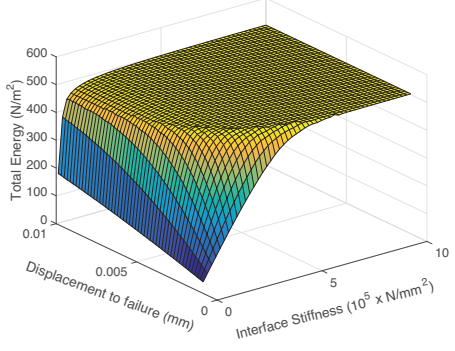


Figure 17: *Interfacial energy dissipated due to debonding is a difficult response surface to sample, due to the large region of almost constant values.*

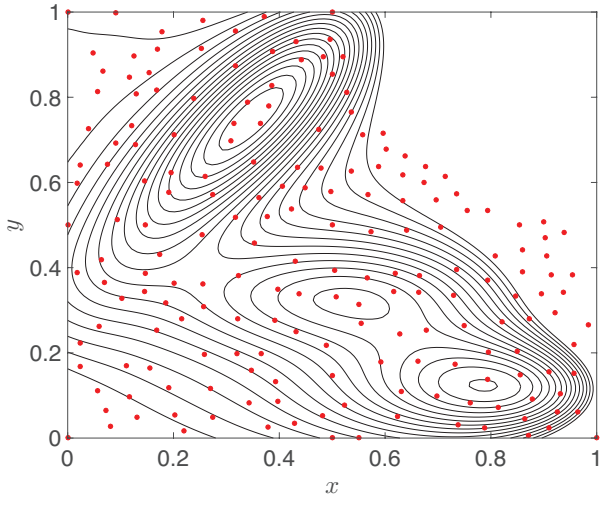


Figure 18: *The Mueller potential is almost exactly reconstructed with a relatively small number of samples, with an algorithm that avoids irrelevant regions such as that in the upper right of the plot.*

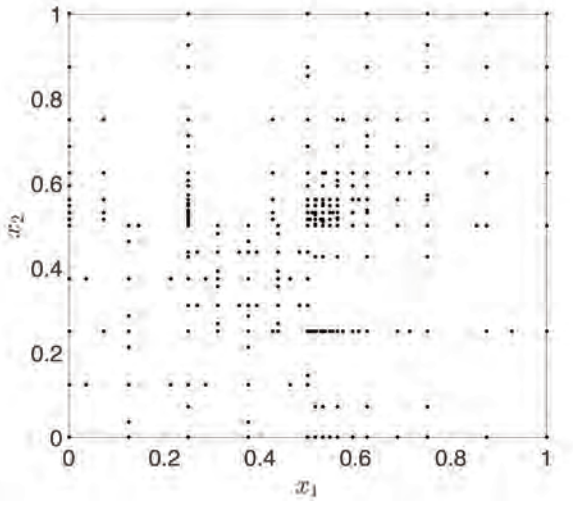


Figure 19: *The adaptive sampling approach developed by the team allows for efficient representation of a discontinuous response function.*

Collaboration Study

Professor Erica Schoenberger
Johns Hopkins University

Collaboration was the organizing principle of the MEDE program from the start. The aim was to make 'materials by design' more innovative by bringing people from different fields together to share ideas, and also much faster by speeding up the 'handoff' between one phase of work and the next.

How do we know if collaboration is working? This is really tough. Collaboration doesn't leave footprints and you can't put it in a TEM. But there are ways of getting a sense of how things are working out. Here I will describe three.

First is the surveys that we have done twice now at the Fall Meeting and will do again at the upcoming one. They are meant to provide descriptive statistics that allow us to see – and to show others – how we are doing the work, what that work produces and how we think about it. Most people feel, for example, that their MEDE work is more collaborative than anything they have done before and also more productive. And with the surveys, we can track changes over time.

Second is interviewing participants about their experience with MEDE. For example, many have stressed that it takes a long time for collaborations to develop and become productive. As one person put it, "Floundering around is actually a healthy start." And here's a comment on the experience of collaboration: "So I could be doing that [work] anywhere and I would be equally happy, right? But it is uniquely satisfying to be part of a team which has this common goal."

Third is watching and listening. I go to meetings large and small. I listen to what people are talking about, how they talk about it, and how they talk to each other.

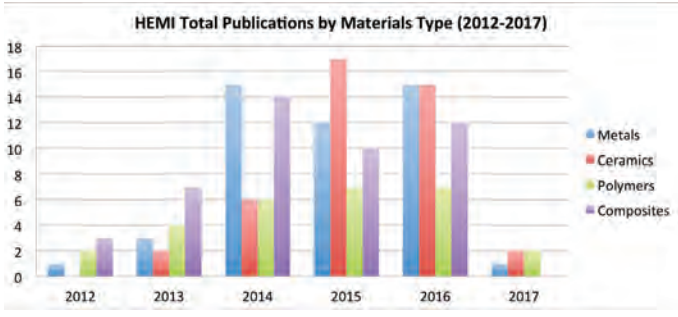
These last two ways of doing research are what I would call quasi-ethnographic. Ethnography is what anthropologists do when they go into the field for a year and a half and live in a village trying to figure out how the people there think about and act in their world. MEDE in a sense is my village.

Some findings:

1. Collaboration means teaching. This may be about substantive issues such as spall or twinning, but the math of different disciplines may also need to be explained. Not that the sums add up differently but, in the words of one respondent: "What groups people to a very large extent is the kind of math they use. If they use different kinds of math, they cannot talk with each other."

2. In many ways the collaborations have worked remarkably well as evidenced by the surveys, the interviews and the papers coming out of the project. . But there is an issue regarding how fast the research moves through what can be thought of as a scientific circuit from theory to synthesis and back again; also how quickly it moves through parallel circuits up and down length and time scales.

3. Third is what I will call alignment, bearing on integration of the research. We might, for example, have a lot of progress in the middle range of the length scale or time scale, but less at either end. Or we might have a lot of computational work at one scale while the experimental work is concentrated at another scale. This could mean that different research tasks aren't lined up correctly to integrate with the prior or following work.



ADDITIONAL COLLABORATIVE ACTIVITIES

Collaborative Research Administration Environment and Data Library (CRAEDL)

Contributed by: Dr. Adam Sierakowski

Beyond its primary scientific mission, the CMEDE consortium faces three key challenges:

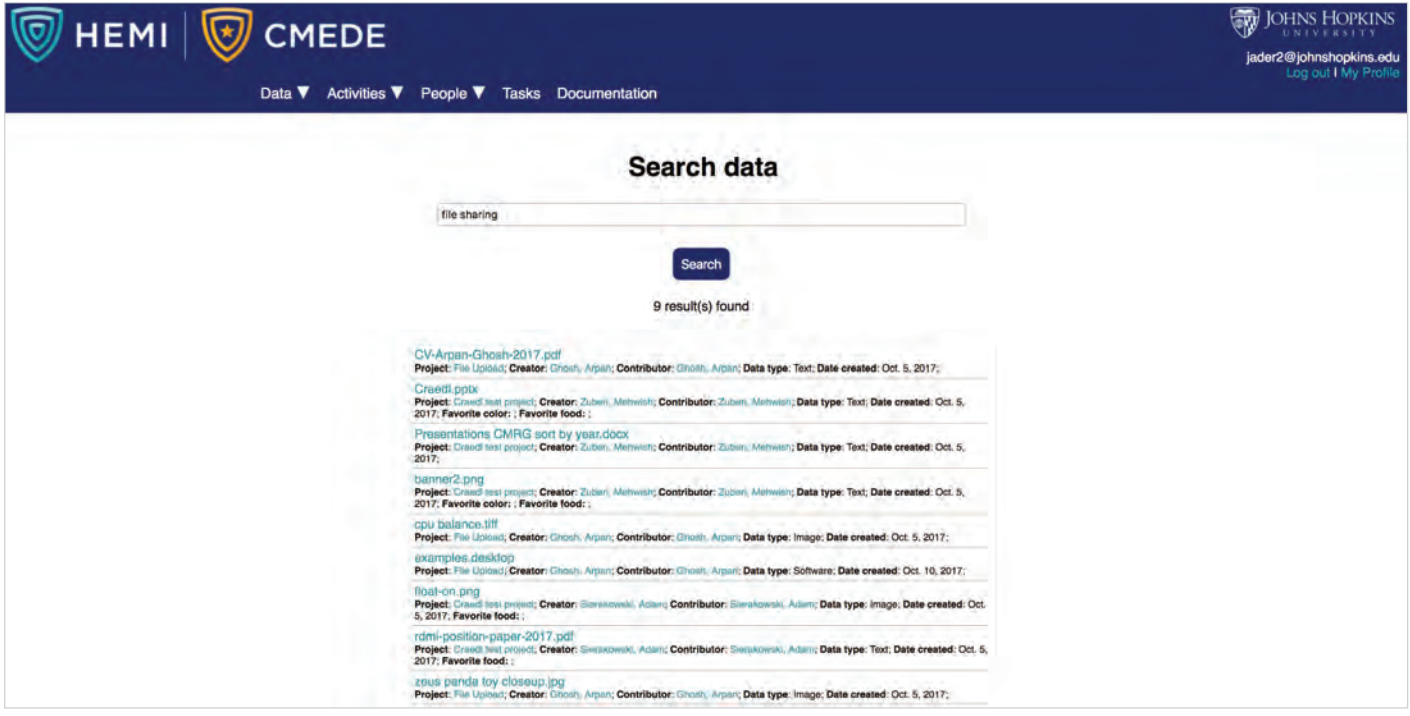
1. Managing the research efforts of hundreds of researchers distributed across the country;
2. Sharing large data sets across institutional boundaries; and
3. Igniting collaborative efforts through data discovery.

Crædl, the Collaborative Research Administration Environment and Data Library, is a tool being developed to overcome these challenges. Accessible at https://hemi.craedl.org, Crædl provides a secure environment for CMEDE affiliates to store their data, share it with collaborators, and search the data shared by other affiliates.

Crædl balances structure and flexibility, enabling researchers to incorporate it directly into their workflow. By doing so, researchers can take advantage of Crædl's automatic metadata population capabilities to document their work in small increments over the life of a project. This metadata — the data that describes the data — is crucially important because it facilitates searching, which prevents data from getting lost and helps colleagues discover otherwise hidden data.Importantly, the researcher maintains complete control over his or her data: All of a researcher's data remains private unless explicitly shared with a collaborator, at which time the data becomes visible to the collaborator's searches.

Researchers log in to Crædl using the credentials of their home institution or with using identity providers. It organizes the network of CMEDE researchers by tracking their grants, projects, data, publications, and presentations to assist in the management of CMEDE's distributed research groups. Crædl facilitates the sharing of large data sets (up to tens of terabytes) using the Globus file transfer service and is currently underpinned by a 350 TB file storage system.

Crædl was released to the MEDE CRA affiliates at the 2017 CMEDE Fall Meeting.



Craedl organized the network of CMEDE researchers to assist in the management of CMEDE's distributed research groups.

ARL Open Campus

The MEDE CRA embraces the ARL Open Campus Initiative. The highly collaborative nature of the MEDE program intrinsically supports consortium members working side by side with ARL scientists and engineers. In addition to taking advantage of ARL's laboratories at Aberdeen Proving Ground in Maryland, CRA members frequently utilize facilities at other MEDE consortium locations. Johns Hopkins University, Rutgers University, and the University of Delaware each have dedicated space for ARL researchers. This promotes the building of a science and technology ecosystem that encourages groundbreaking advances in basic and applied research areas of relevance to the Army.

UK Collaboration with the MEDE Programme

Contributed by: Laura Jones CEng FIMMM

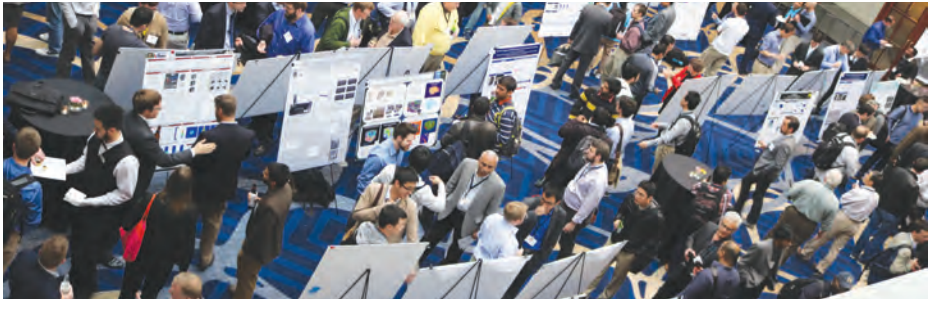
The UK Ministry of Defence at the Defence Science and Technology Laboratory (Dstl) funds a major materials research activity. Historically known as MAST, this has recently become the Materials for Strategic Advantage (MSA) Programme. In the new Programme, a significant focus remains the behaviour of materials under high strain rate. Specifically, the new Programme has a requirement to develop robust materials for the protection of the dismounted soldier and land vehicles. Collaboration with the US is seen as vital in advancing the state of the art in this important area of science and technology.

The MEDE Program is pivotal to enabling collaboration between the UK and US in this area of materials science. Dstl staff will attend the Fall Meeting in Baltimore and will hopefully be presenting work of interest to the MEDE community during the spring as well. An emerging and potentially disruptive area of science and technology that now falls within the MSA Programme is that of synthetic biology. The UK is investing heavily in the application of synthetic biology to enable the next generation of materials for physical protection, including funding work on silicon carbide and transparent armour. The opportunity exists to expose some of these developments to the MEDE community, along with developments in the UK of more traditional materials science aimed at providing a step change in the performance of physical protection solutions.

The UK MSA Programme looks forward to a fruitful and ongoing relationship with MEDE.

MEDE Fall Meeting

The MEDE Fall Meeting is an annual, closed event that brings the entire MEDE CRA together for program overviews, collaborative activities and discussion. In 2017, the event was attended by 136 individuals including special guests from the United Kingdom's Defence Science and Technology Laboratory; Army Research Office; Natick Soldier Research, Development and Engineering Center; US Army Engineer and Development Center and members of the MEDE science advisory board. Professor K.T. Ramesh (JHU) and Dr. John Beatty (ARL) led the meeting, which focused on technical collaboration across the MEDE CRA and program planning for the upcoming year.



Mach Conference

The Mach Conference is an annual, open event that showcases the state of the art of multiscale research in materials, with an emphasis on advancing the fundamental science and engineering of materials and structures in extreme environments. MEDE CRA members are significant participants in this event, which shares research discoveries to the broader community.

SIGNIFICANT MEETINGS

EMRM Mid-Cycle Review

On February 16, 2017, the ARL Chief Scientist hosted a review of the Enterprise for Multiscale Research of Materials (EMRM) at the Adelphi Laboratory Center. Attendees included senior technical representatives from ARL and the Deputy Chief Scientist from the Office of the Assistant Secretary of the Army for Acquisition, Logistics and Technology. The review focused on technical and programmatic updates on the MEDE and MSME CRAs.

MEDE Science Advisory Board

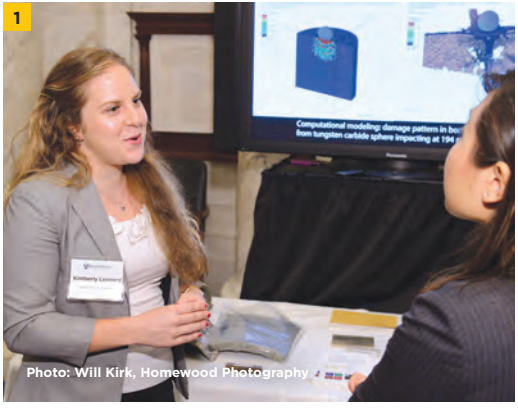
The MEDE Science Advisory Board is convened annually to review the scientific and collaborative activities within the program. The Board's recommendations in coordination with those from ARL's Technical Advisory Board are used to help prioritize research activities and shape the overall program.

Hopkins on the Hill

On June 13, 2017, JHU presented the MEDE CRA at the Hopkins on the Hill event which was held in the Russell Senate Office Building in Washington, DC. The purpose of this event was to inform members of Congress and their staff of the importance of federal funding in supporting the MEDE CRA. This event was highlighted by Senators Ben Cardin (D-MD) and Chris Van Hollen (D-MD) participating in the event activities.

Magnesium Workshop

On April 3-4, 2017, the Hopkins Extreme Materials Institute hosted a two-day, invitation-only workshop focused on magnesium. Leading experts from the United States, Japan, Australia, and Germany traveled to the Homewood campus of Johns Hopkins University to discuss the current state of the art in magnesium experiments, modeling and simulation, processing and design. The workshop included representatives from the Army Research Laboratory due to their specific interest in magnesium as a protection material for military applications.



1. *JHU graduate student Kimberly Leonard speaks about her research during Hopkins on the Hill*

2. *JHU President Ronald J. Daniels looks on as Senator Benjamin Cardin (D-MD) speaks at the Hopkins on the Hill event*

3. *Magnesium workshop presenters*

RELATED ACADEMIC PROGRAMS

In addition to its research activities, CMEDE runs several academic programs that broaden the scientific impact of the MEDE program.

Traditional

- Short Courses – Intensive, two-day courses taught by a master in his/her field that are co-sponsored by the Hopkins Extreme Materials Institute. Attendees include professionals, researchers, and graduate students from industry, government, national laboratories and academia.

- Lectures and Seminars – CMEDE supports the Enterprise for Multiscale Research of Materials lecture series that helps to educate and promote collaboration across the entire enterprise. Additionally, CMEDE hosts seminars from distinguished experts from scientific fields related to MEDE research.

Figure 20: *Prof. Sung Hoon Kang hosts a seminar on additive manufacturing*

Internships and Apprenticeships

- Extreme Science Internships (ESI) – The ESI program is a year-round, paid internship program with Morgan State University. ESI provides internal internships at Morgan State to allow students to develop their research skills before participating in an external internship at a MEDE CRA location. ESI has been a highly successful program and serves as a model collaboration for student development.

- Undergraduate Research and Apprenticeship Program (URAP). URAP provides undergraduate students with an authentic science and engineering research experience alongside university researchers at one of the MEDE university locations. Through this program, students develop skills in Army critical science and engineering research areas to prepare them for the next steps of their educational and professional career. URAP is sponsored by the Army Research Office and is a part of the Army Educational Outreach Program.

- Research and Engineering Apprenticeship Program (REAP). The Hopkins Extreme Materials Institute (HEMI), parent to CMEDE at Johns Hopkins University, was selected as a host site for REAP. REAP is a summer STEM program that places talented high school students, from groups historically under-represented and underserved, in STEM in research apprenticeships. REAP apprentices work under the direct supervision of a mentor on a hands-on research project. REAP is a part of the Army Educational Outreach Program.

Figure 21: *URAP intern Alexa Herrera works with boron carbide during her internship at Rutgers University*

Other Activities

- In 2016-17, the Hopkins Extreme Materials Institute was awarded an Army Educational Outreach Program (AEOP) Strategic Outreach Initiatives grant. The grant helps to promote AEOP opportunities and STEM programs sponsored by Johns Hopkins University's Center for Educational Outreach, with a particular focus on Baltimore City schools and military families stationed at Aberdeen Proving Ground and Adelphi Laboratory Center locations. CMEDE's involvement with AEOP demonstrates a commitment to supporting the U.S. Army's strategic goals for promoting STEM activities and the next generation work force.

- HEMI/MICA Extreme Arts Program – The HEMI/MICA Extreme Arts Program is a new initiative that brings faculty and students from Johns Hopkins University and the Maryland Institute College of Art (MICA) together to explore unique perspectives on extreme events. The program aims to encourage collaboration among artists and researchers to examine data, interpret outcomes, and translate results from extreme events in new ways. It is our hope that this dialogue will create a stronger community through a shared sense of curiosity and exploration. CMEDE is a significant participant in this program.

Figure 22: *2017 AEOP Research in Engineering Apprenticeship students with representatives from AEOP and the U.S. Army Research Office*

CMEDE STRATEGIC PARTNERSHIPS

MEDE has established strategic partnerships with several key organizations. These partnerships enable CMEDE to collaborate, leverage resources and broaden its impact to the scientific community.

Subcommittee of the Materials Genome Initiative (SMGI) of the National Science and Technology Council

Center for Composites Materials (CCM)

Army Educational Outreach Program

US Advanced Ceramics Association (USACA)

The Insitute for Data Intensive Engineering and Science

Center of Excellence on Intergrated Materials Modeling

Maryland Advanced Research Computing Center (MARCC)

Lightweight Innovations for Tomorrow (LIFT)

Ceramics, Composite and Optical Materials Center (CCOMC)

U.S. Naval Research Laboratory

National Institutes of Standards and Technology

CMEDE LEADERSHIP AND STAFF MEMBERS AT JOHNS HOPKINS UNIVERSITY

CMEDE Leadership

Prof. K.T. Ramesh
Director

Prof Lori Graham-Brady
Associate Director

Dr. Victor Nakano
Executive Program Director

CMEDE Staff

Jessica Ader
Communication Specialist

Bess Bieluczyk
Senior Administrative Coordinator

Tia Brownlee
Budget Analyst

Angela Coleman
Budget Analyst

Scott McGhee
Senior Administrative Manager

Phyllis Sevik
Research Service Manager

Matthew Shaeffer
Staff Engineer

Dr. Adam Sierakowski
Assistant Research Scientist

Katie Vaught
Senior Administrative Coordinator

Mehwish Zuberi
Junior Database Administrator

ABBREVIATIONS AND ACRONYMS

ARL	Army Research Laboratory
AEOP	Army Educational Outreach Program
CALTECH	California Institute of Technology
CCM	Center for Composite Materials
CCOMC	Ceramic, Composite and Optical Materials Center
CEIMM	Center of Excellence on Integrated Materials Modeling
CMC	Consortium Management Committee
CMEDE	Center for Materials in Extreme Dynamic Environments
CMRG	Collaborative Materials Research Group
CTRG	Collaborative Technical Research Group
CRA	Collaborative Research Alliance
CRAEDL	Collaborative Research Administration Environment and Data Library
DELAWARE	University of Delaware
DOD	Department of Defense
DREXEL	Drexel University
DSTL	Defence Science and Technology Laboratory
EMRM	Enterprise for Multiscale Research of Materials
ESI	Extreme Science Internship
HEMI	Hopkins Extreme Materials Institute
JHU	Johns Hopkins University
MEDE	Materials in Extreme Dynamic Environments
MEDE CRA	MEDE Collaborative Research Alliance
MGI	Materials Genome Intitative
MICA	Maryland Institute College of Art
MSU	Morgan State University
NC A&T	North Carolina Agricultural & Technical State University
NIST	National Institute of Standards and Technology
NMT	New Mexico Institute of Mining and Technology
PURDUE	Purdue University
REAP	Research in Engineering Apprenticeship Program
RMB	Research Management Board
RUTGERS	Rutgers University
STEM	Science, Technology, Engineering and Math
UHMWPE	Ultra High Molecular Weight Polyethylene
UNCC	University of North Carolina at Charlotte
URAP	Undergraduate Research and Apprenticeship Program
UTSA	The University of Texas at San Antonio

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For more information on CMEDE, visit us at: hemi.jhu.edu/cmede, call us at 410-516-7257 or email us at mede@jhu.edu.

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