HIGHLIGHTS 2015

CMEDE

CENTER FOR
MATERIALS IN EXTREME
DYNAMIC ENVIRONMENTS

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 creates a collaborative environment within which partners from academia, government, and industry 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 first in an annual series of highlights from the Center for Materials in Extreme Dynamic Environments (CMEDE).

The Center is a collaborative effort between a consortium of fifteen research institutions, led by the Johns Hopkins University, and the U.S. Army Research Laboratory. CMEDE was established in 2012 with two goals: advancing the fundamental understanding of materials in extreme dynamic environments, and developing a materials-by-design capability for protection materials. Our approach is unique both in the degree of multi-disciplinarity and in the degree of collaboration that is integral to our efforts.

This 2015 issue of our Highlights describes the unique aspects of our activities, and showcases a small sampling of the programs and people within each of our materials research groups (ceramics, composites, metals, and polymers). These achievements are exciting because they have broad and deep impacts on our scientific and technological capabilities, as well as developing a new workforce educated in the exciting possibilities of materials-by-design. We are positive that the advances we are making in the science and the workforce will have great impact on the protection of our military personnel and vehicles.

We are very grateful for the continued support of the U.S. Army and the Department of Defense, as well as the support of many partners within the Enterprise for Multiscale Research of Materials and the MEDE Collaborative Research Alliance. The quality and extent of the research and collaborative activities described here would not be possible without the support of all of these agencies and organizations.

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Science & Engineering

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ABOUT US

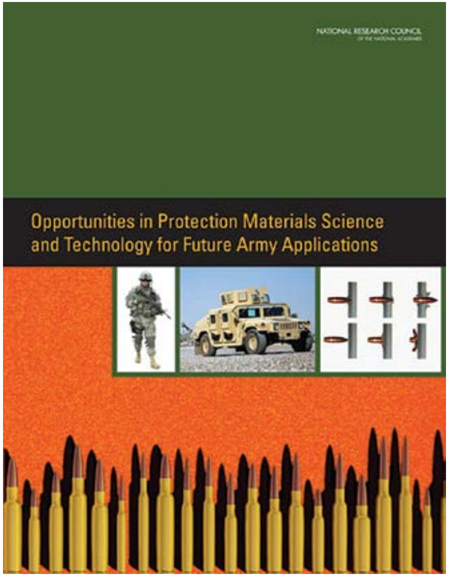
In 2010, two National Research Council boards established a committee to examine opportunities in protection materials science and technology for future Army applications. This committee recommended that the Department of Defense should establish an initiative for protection materials by design. This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

In response to the committee's recommendation, in April 2012 the Army Research Laboratory (ARL) established a framework to integrate all of 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 US 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 Enterprise 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



NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

Opportunities in Protection Materials Science and Technology for Future Army Applications

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 ten-year agreement, valued up to $90 million, represents a significant investment and demonstrates the importance of the design of protection materials to the US Army.

"In our Basic Research portfolio we are pursuing a number of potentially game-changing technologies. Our 'Materials on Demand and By Design' research will provide the capability to select and create material properties and responses, essentially building new materials from the atom up. This effort requires intensive computational capability and the research to establish (and validate) a model that accurately reflects the material properties across the various domains from the atom to the continuum. The result is a materials-by-design capability for ballistic protection, energetic materials and electronic materials, built using a multiscale approach heavily leveraging computational materials science."

Statement by Ms. Mary Miller, Deputy Assistant Secretary of the Army for Research and Technology to a House Appropriations subcommittee, March 26, 2015.

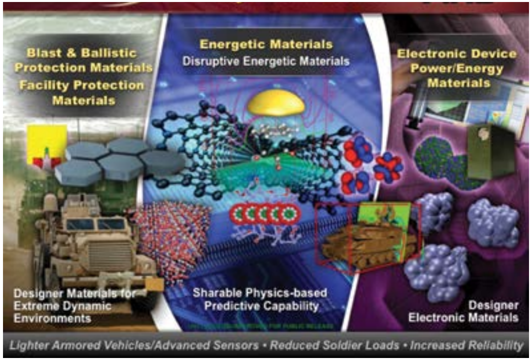


Figure 2: *Army illustration depicting EMRM.*

In addition to supporting the US 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 government's largest investments in extramural basic research in support of the Materials Genome Initiative.

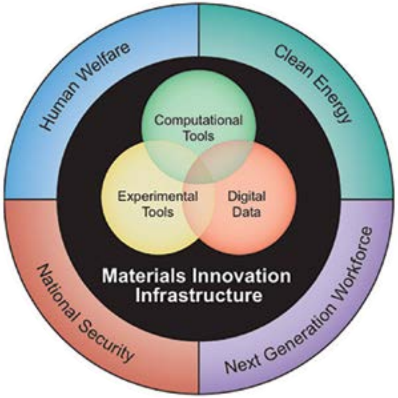


Figure 3: *Materials Genome Initiative: MEDE focuses on developing the experimental and computational tools needed to develop protection materials for national security.*

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**
- **Lawrence Livermore National Laboratory**
- **Morgan State University**
- **New Mexico Institute for Mining and Technology**
- **Purdue University**
- **Southwest Research Institute**
- **University of California, Santa Barbara**
- **University of Texas at San Antonio**
- **Washington State University**

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

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UNIVERSITY OF DELAWARE

PURDUE UNIVERSITY

RUTGERS

SwRI

Drexel UNIVERSITY

UCSB

Lawrence Livermore National Laboratory

UTSA

MORGAN STATE UNIVERSITY

WASHINGTON STATE UNIVERSITY

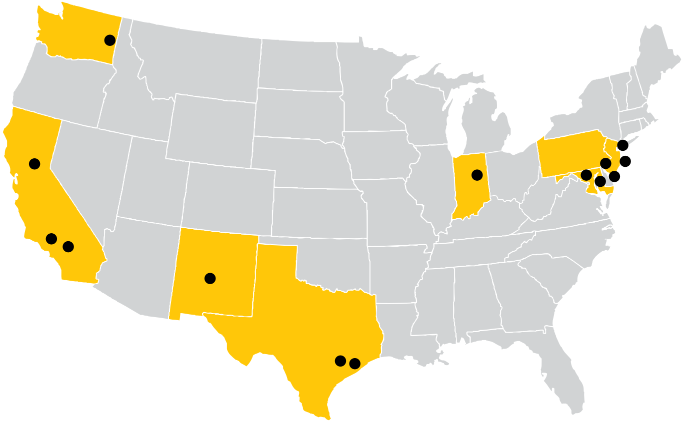


Figure 4: *MEDE Collaborative Research Alliance*

United Kingdom

[dstl]

Germany

Fraunhofer EMI

STRUCTURE

- The CMEDE Director is located within CMEDE at Johns Hopkins University, since JHU is 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 are three Collaborative Technical Research Groups (CTRGs): experimental, modeling and processing. Each CTRG is co-led by a consortium principal investigator and an ARL researcher.

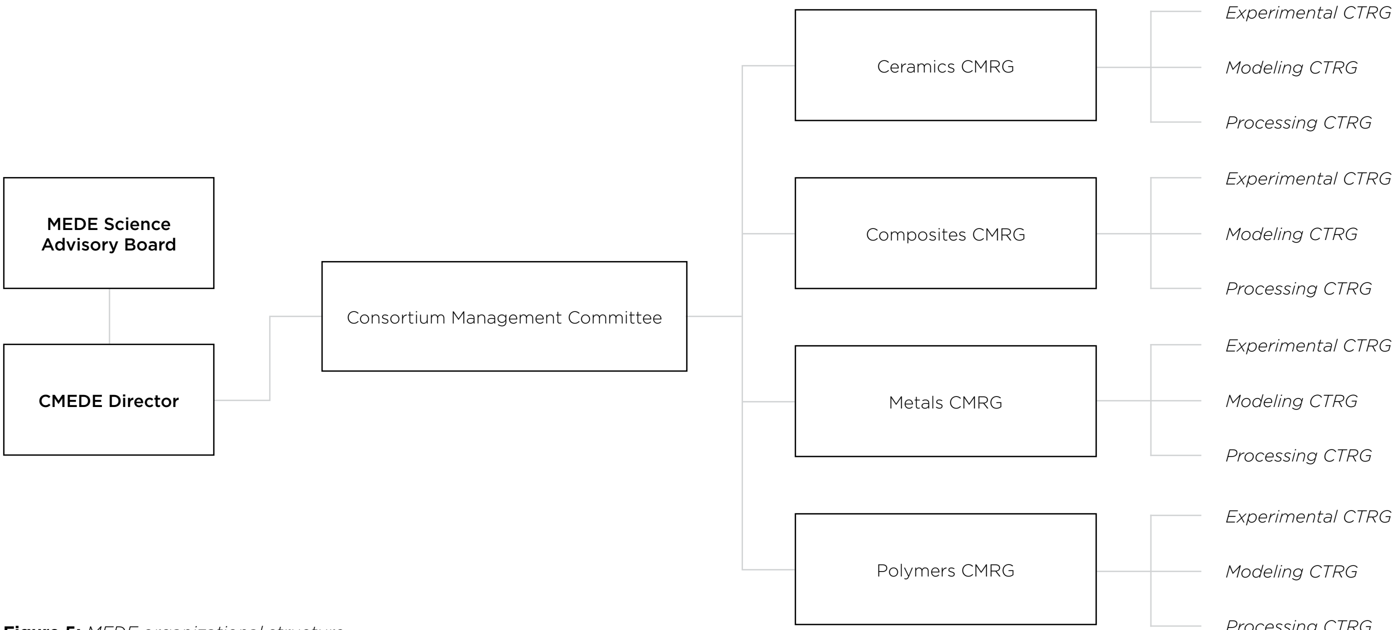


Figure 5: *MEDE organizational structure*

From left: Prof. Steve McKnight, Virginia Tech; Prof. Rodney Clifton, Brown University; Dr. Donald Shockey, SRI International; Prof. Susan Sinnott, Penn State; Prof. David McDowell, Georgia Tech; Dr. Doug Templeton, DWT Consulting; Dr. John Beatty, U.S. Army Research Laboratory; Prof. KT Ramesh, Johns Hopkins University. Not shown: Prof. Marc Meyers, UC San Diego; Prof. Tony Rollett, Carnegie Mellon University; and Prof. Tom Russell, University of Massachusetts Amherst.

MEDE SCIENCE ADVISORY BOARD MEMBERS

- Dr. Donald Shockey, SRI International (Chair)
- Professor Rodney Clifton, Brown University
- Professor David McDowell, Georgia Institute of Technology
- Professor Steve McKnight, Virginia Polytechnic Institute
- Professor Marc Meyers, University of California, San Diego
- Professor Tony Rollett, Carnegie Mellon University
- Professor Tom Russell, University of Massachusetts Amherst
- Professor Susan Sinnott, Pennsylvania State University
- Dr. Doug 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 6. 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 their 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. We 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. Similarly, controlling the mechanism through synthesis and processing leads to new designed materials for the canonical environment. Industry helps to determine the scale-up feasibility of these new designed materials which are then fed back to the experiments in the canonical modeling effort.

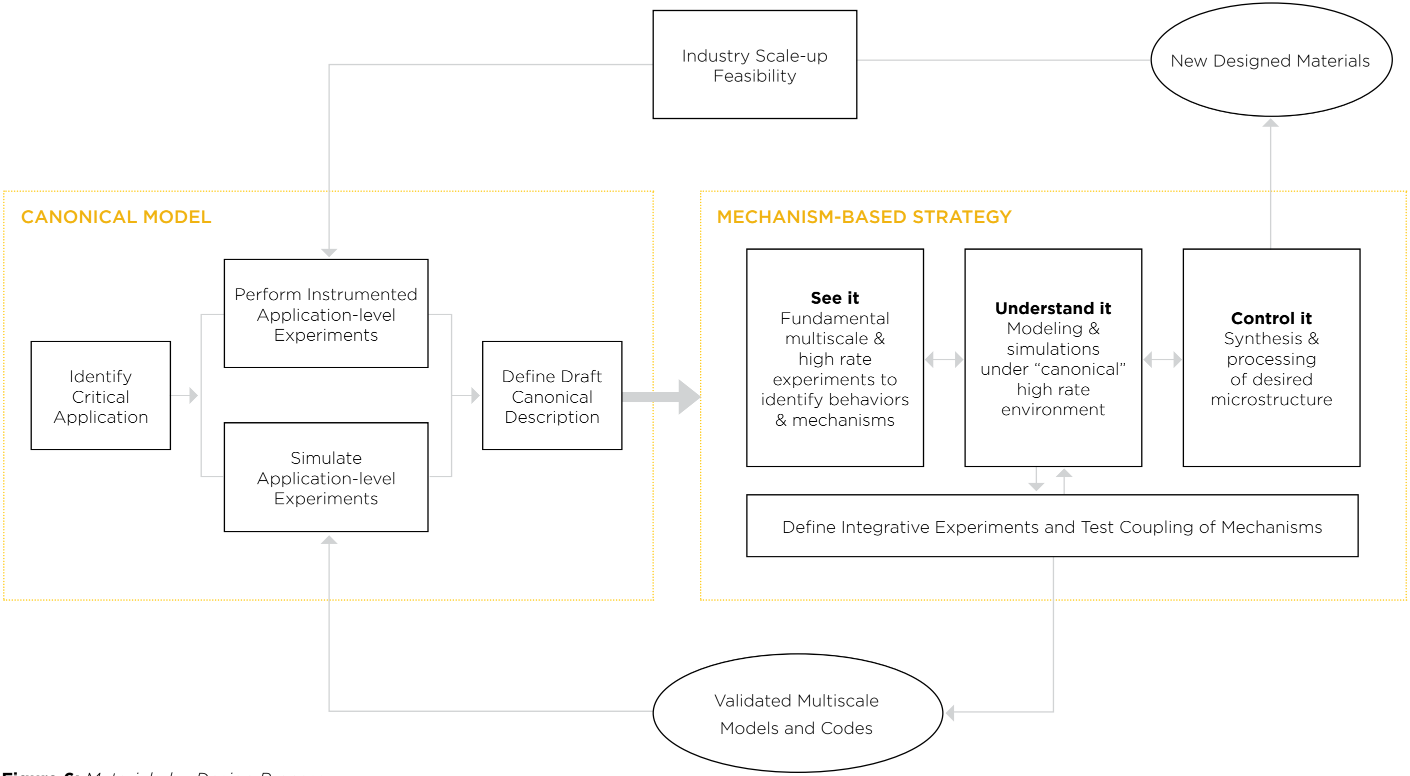


Figure 6: *Materials-by-Design Process*

RESEARCH ACTIVITIES

Currently the MEDE program examines one model material in each of the following four material classes: ceramics, composites, metals, and polymers. The 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 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 Interface

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.

Metals: Magnesium

The magnesium alloy system is the model material for the Metals CMRG because this 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 US 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 ARE ORGANIZED BY 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.

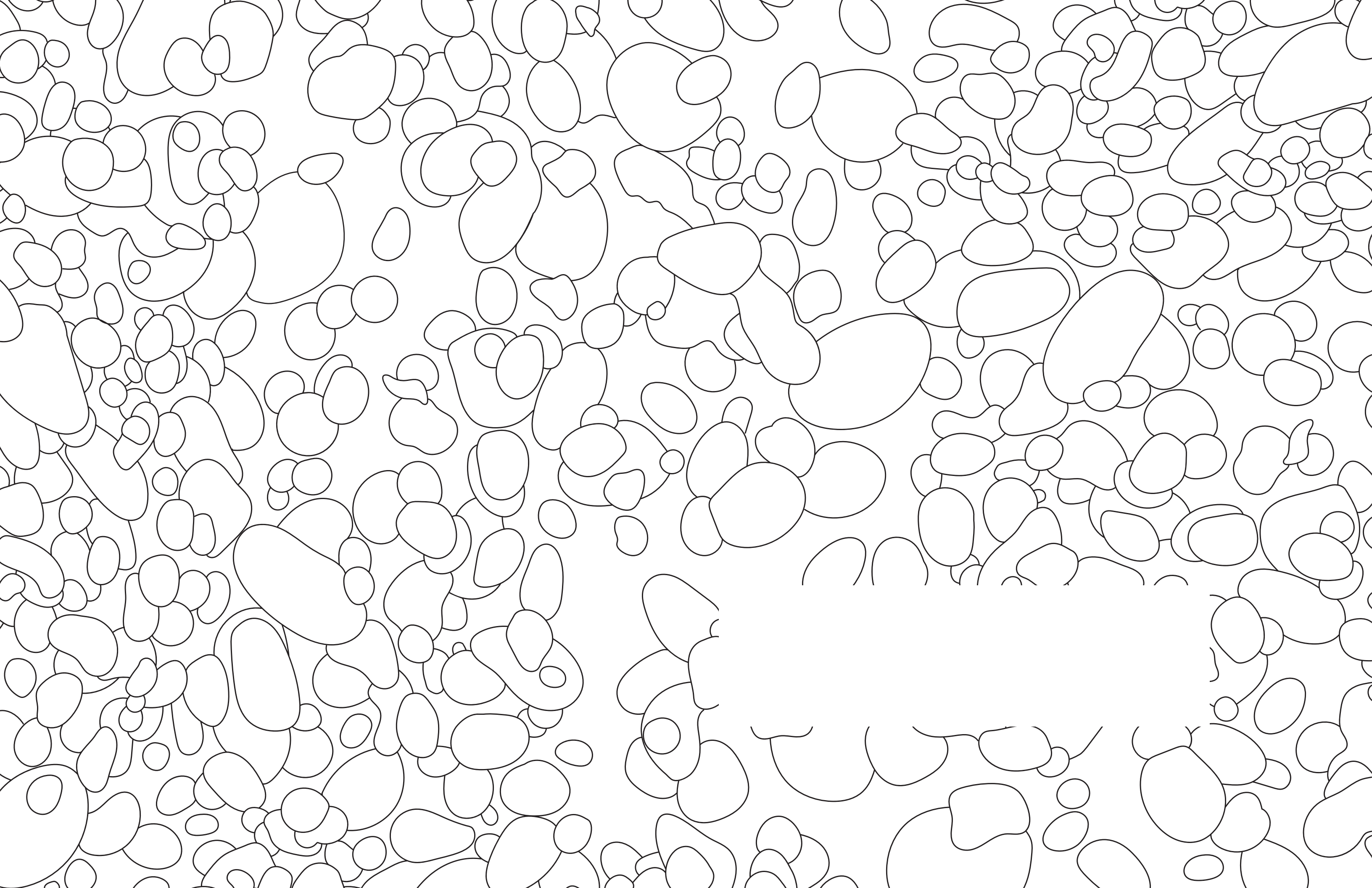
- **Modeling and Simulation:** developing computational approaches to predict the materials response to extreme dynamic environments at critical length and time scales.

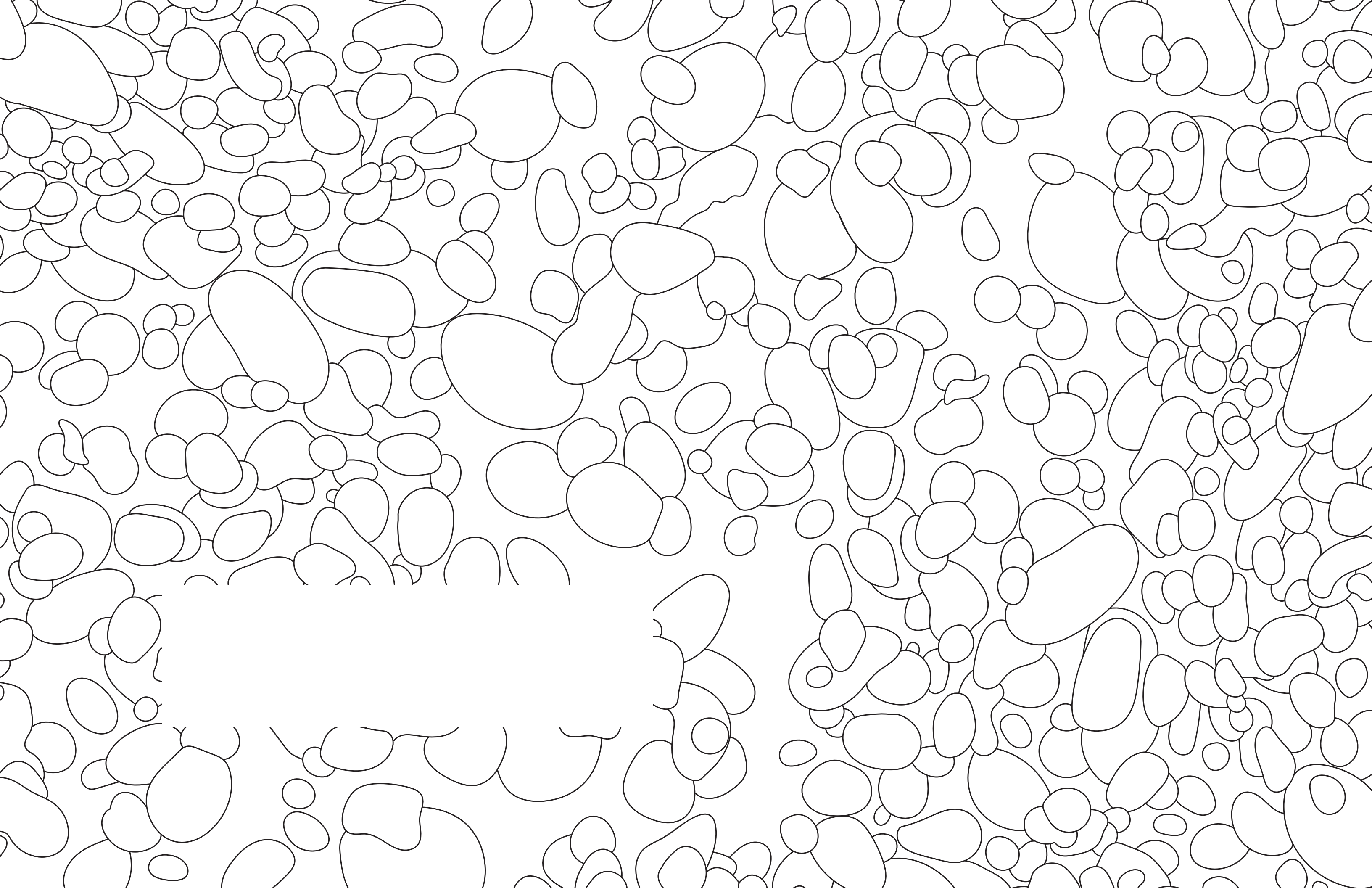
- **Bridging the Scales:** developing physical and mathematical constructs necessary to bridge critical length and time scales.

- **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

Dr. Charles Anderson, SwRI

Prof. Nitin Daphalapurkar, JHU

Dr. Vlad Domnich, Rutgers

Prof. William Goddard, Caltech

Prof. Lori Graham-Brady, JHU

Prof. Rich Haber, Rutgers

Prof. Kevin Hemker, JHU

Mr. Tim Holmquist, SwRI

Prof. Bob McMeeking, UCSB

Prof. K.T. Ramesh, JHU

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Dr. Sikhanda Satapathy

Dr. Brian Schuster

Dr. JP Singh

Dr. Jeffrey Swab

Dr. Jennifer Synowczynski-Dunn

Dr. DeCarlos Taylor

Dr. Andrew Tonge

CONSORTIUM RESEARCH TASKS

- In situ visualization in Kolsky bar experiments (Ramesh, JHU)
- TEM characterization of boron carbide (Hemker, JHU)
- Physics-Based Constitutive Models for Intact and Damaged Advanced Ceramics (Graham-Brady, Ramesh and Daphalapurkar; JHU, McMeeking; UCSB)
- Development of ReaxFF reactive force field for boron carbide (Goddard, Caltech)
- Characterization of boron carbide powders and boron carbide ceramics (Haber and Domnich, Rutgers)
- Synthesis and processing of enhanced boron carbide (Haber, Rutgers)
- Incorporating MEDE material models into EPIC (Anderson and Holmquist, SwRI)

Atomistic Origin of Brittle Failure of Boron Carbide from Large Scale Reactive Dynamics Simulations; Suggestions toward Improved Ductility

Dr. Qi An
California Institute of Technology

Professor William A. Goddard III
California Institute of Technology

Ceramics are strong, but their low fracture toughness prevents extended engineering applications. In particular, boron carbide, the third hardest material in nature, has not been incorporated into many commercial applications because it exhibits anomalous failure when subjected to hypervelocity impact. To determine the atomistic origin of this brittle failure, we have performed large-scale (~200,000 atoms/cell) reactive-molecular-dynamics simulations of shear deformations of boron carbide, using the quantum-mechanics-derived ReaxFF reactive force field. We have examined the (0001)/<1010> slip system related to deformation twinning and the (0111)/<1101> slip system related to amorphous band formation.

Our simulations and analysis of the failure process show that **the origin of the brittle failure fracture for boron carbide is the formation of higher density amorphous bands** that lead to negative pressures, cavitation, and eventually crack opening. The high density of the amorphous structures was further confirmed by the ab initio molecular dynamics (AIMD) simulations.

Thus, to design ductile materials based on boron carbide we are considering alloying aimed at promoting shear relaxation through inter-icosahedral slip that avoids icosahedral fracture.

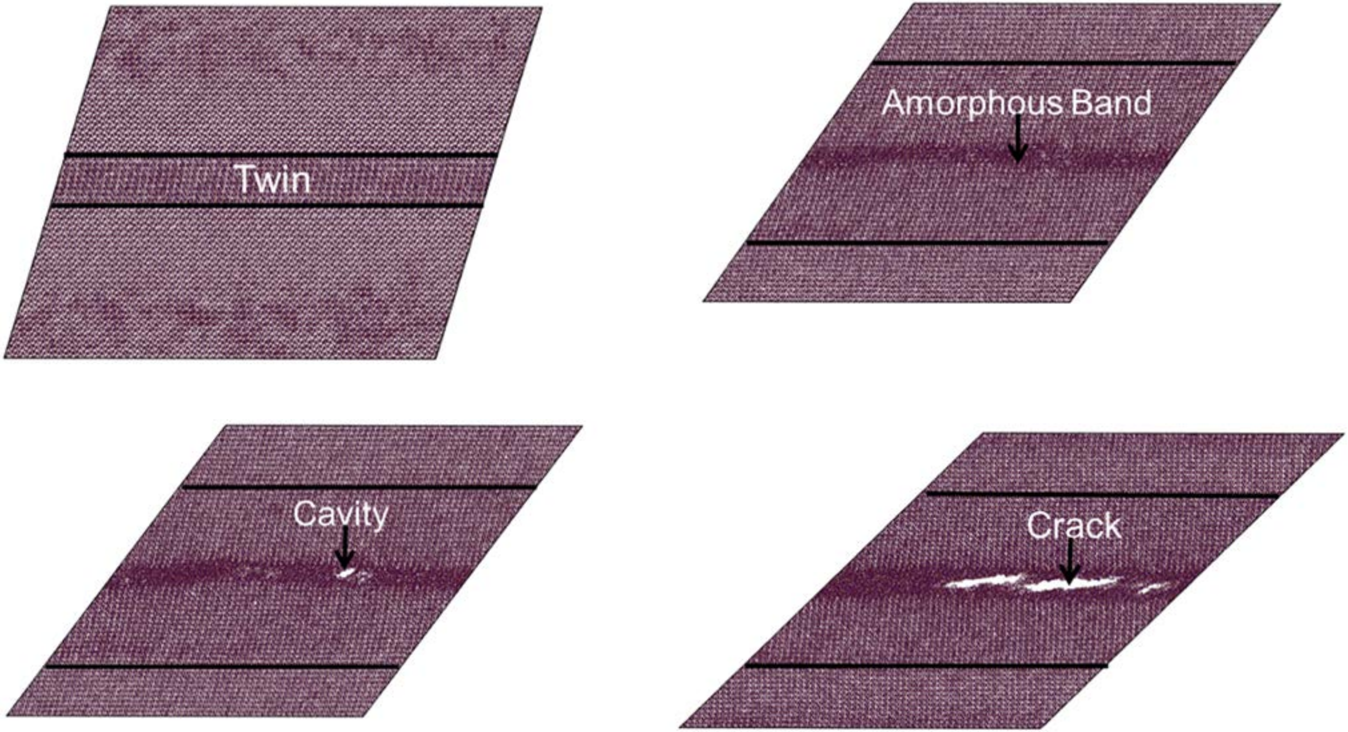

Figure 7: *Atomistic simulations of amorphization in boron carbide.*

Dynamic Failure of Advanced Ceramics: Modeling and Codes

Dr. Andrew Tonge
Army Research Laboratory

Professor K.T. Ramesh
Johns Hopkins University

Dr. Richard Becker
Army Research Laboratory

Dr. Betsy Rice
Army Research Laboratory

Mr. Tim Holmquist
Southwest Research Institute

The design of revolutionary armor ceramics cannot be accomplished without an understanding of the particular combinations of failure mechanisms that arise within these materials. We have developed a physics-based material model where each failure mechanism in the model is linked to a set of microstructural parameters. These mechanisms include viscous heating through shock formation, elastic softening as a result of micro-crack growth, granular flow of the fully damaged material, and plasticity. Using this model, we have examined the relative importance of each energy dissipation pathway for a variety of loading conditions. Insights from this investigation suggest promising directions for future effort in the development of improved advanced ceramics.

The Tonge-Ramesh (TR) model includes physically based material variability, micromechanics-based damage growth, granular flow, compaction of the granular material, and a selected equation of state. Using this new modeling framework, we have simulated a variety of experimental configurations and armor ceramic materials, and have provided guidance to synthesis and processing for the generation of much-improved materials. Through simulations of simplified ballistic impact on boron carbide, for example, we demonstrate (Figure 8) that the extent of granular flow and material microcracking is linked to the granular flow surface slope, suggesting that materials capable of forming larger, high aspect ratio fragments may provide better resistance to penetration.

The TR model was developed in the Uintah software suite, a set of libraries and applications for simulating and analyzing complex chemical and physical reactions. The TR model was transitioned to a form that allows it to be rapidly integrated into codes relevant to the application environment with the help of Dr. Richard Becker (ARL), Dr. Betsy Rice (ARL), Mr. Timothy Holmquist (SwRI), and ARL's supercomputing resource center.

The TR model in Uintah is available in the public domain to enhance broad research in advanced ceramics.

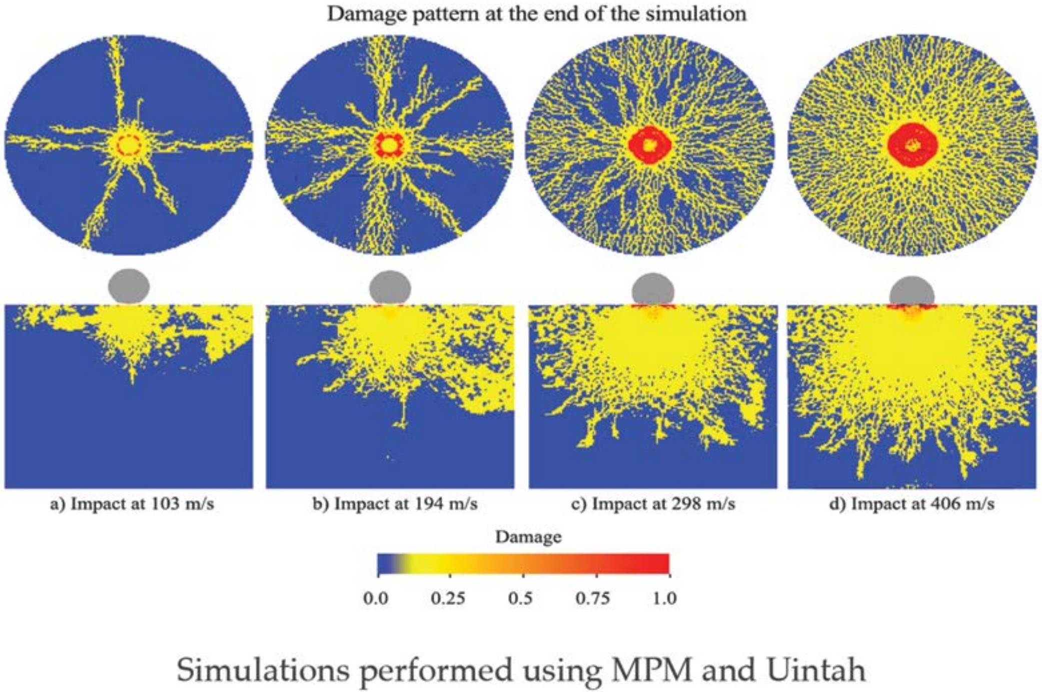

Figure 8: *Simulations of the failure of a boron carbide target impacted by hard sphere.*

RESEARCHER HIGHLIGHT: ANDREW 'ANDY' TONGE

Andy began his work with the MEDE program as a student at Johns Hopkins University. Upon receiving his Ph.D., Andy was hired by the Army Research Laboratory. He is currently facilitating the integration of the MEDE developed models into production simulation codes where they can provide greater impact to the Army. Part of this effort is exercising the material models in simulations of the integrated experiments.

How did you get involved with the MEDE program?
I came to Hopkins looking to study composite materials building on some of the undergraduate research that I had done looking at thermoplastic/s-glass composites for protection applications. K.T.'s group's focus on dynamic deformation mechanisms attracted me to the group. After joining the group, I spent some time looking at boundary effects in single crystal quartz experiments and using SPH for simulations of meteorite impact. I realized that, while there was significant work to be done on numerical methods (like SPH), the strength of the group and the expertise that I had around me was better suited to developing improved material models for high rate impact events. As I was developing my material model for dynamic brittle failure (with applications to both geologic materials and armor ceramics) the MEDE program was forming. Once the MEDE program was fully operational, it was a natural fit for my research area.

What are your current activities with MEDE?
I am a researcher at ARL facilitating the integration of the MEDE developed models into production simulation codes where they can provide greater impact to the Army. Part of this effort is exercising the material models in simulations of the integrated experiments.

What would you consider some of your biggest accomplishments?
Developing a model that bridges microstructural characterization and structural simulation for ceramic materials then incorporating the model into several simulation codes. Additionally, in 2014 I was recognized as a Future Leader by the American Ceramics Society as a part of the Future Leaders Program at the Ceramics Leadership Summit, and in 2012, I received an Alex Charters Scholar award from the Hyper Velocity Impact Society.

Who are your biggest influences in both your personal and professional life?
Professionally - Professor K.T. Ramesh. He taught me to think about research problems in terms of the mechanisms that are active and the processes that those enable. This is an approach that will allow me to look at many types of problems throughout my research career. Also Larry Parent, who was an advisor for my undergraduate research and encouraged me to pursue graduate research after spending some time in industry.

Personally - My wife Theresa who shared the Ph.D. journey with me and has continued to support my endeavors. Additionally, my grandparents have been large influences on my life, especially Russ Haris and Bob Koucky who from a young age always encouraged me to explore the natural world and seek to understand it through the eyes of an engineer.

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 O'Brien

Composites CMRG

CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Cameron Abrams, Drexel

Prof. Suresh Advani, Delaware

Prof. Kadir Aslan, Morgan State

Prof. Somnath Ghosh, JHU

Prof. John W. Gillespie, Jr., Delaware

Prof. Lori Graham-Brady, JHU

Prof. Bazle Haque, Delaware

Prof. Giuseppe Palmese, Delaware

Prof. Shridhar Yarlagadda, Delaware

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Dr. Travis Bogetti

Dr. Robert Elder

Dr. Joe Lenhart

Dr. Kevin Masser

Mr. Chris Meyer

Dr. Danny O'Brien

Dr. James Sands

Dr. Timothy Sirk

Dr. Tusit Weerasooriya

Dr. Chian Fong Yen

CONSORTIUM RESEARCH TASKS

- High-rate test methods for interphase characterization (Gillespie and Haque, Delaware)
- Multi-scale modeling of fiber-matrix interphase (Haque and Abrams, Delaware)
- High strain-rate fiber-matrix interfacial traction laws (Gillespie and Keefe, Delaware)
- Synthesis and characterization of model interphases and tows with controlled resin distribution (Advani and Yarlagadda, Delaware)
- Multi-scale damage modeling of composites (Ghosh, JHU)
- Epoxy molecular simulations (Abrams, Drexel)
- Synthesis and characterization of epoxy networks with controlled topology (Palmese, Drexel)
- Characterization of damage in S2 glass/epoxy system (Aslan, Morgan State)

Fiber-Matrix Interphase by Design

Professor Bazle Haque
University of Delaware

Professor John W. Gillespie, Jr.
University of Delaware

The fiber-matrix interphase plays a critical role in stress wave propagation, load transfer, and energy dissipation during micro-mechanical fiber fracture, interphase debonding, and matrix-cracking under extreme dynamic loading conditions. Molecular dynamics (MD) models of glass-fibers (SiO_2), interphase sizing compound (GPS silane & epoxy), and the epoxy-amine matrix network have been developed to predict the rate-dependent properties and to understand the failure behavior of these constituent materials. The chemical composition and network structure of the interphase material greatly affects the chemical bonding to the glass surface and to the epoxy-amine matrix network. Figure 9 shows MD simulations of the fiber-matrix interphase. Such models have been subjected to dynamic loading under Mode I, Mode II, and Mixed-mode loading conditions to quantify the traction-separation behavior of the interphase. This has also been used to determine the parameters of a potential-based cohesive zone model (PPR-CZM), which is used at the next scale up. A high-strain-rate micro-droplet interphase test method has also been developed, and different fiber-matrix interphases have been characterized at a wide range of strain rates from near quasi-static to high strain-rates (up to 10^8 s^{-1}). Finite element models of the dynamic micro-droplet experiments have been developed and simulated to determine a unique cohesive zone model (CZM) based on initiation and propagation of a crack in the fiber-matrix interphase. We expect that our MD predictions of the parameters of the potential based interphase traction-separation behavior will enable the design of a fiber-matrix interphase for optimum energy dissipation under extreme dynamic loading condition.

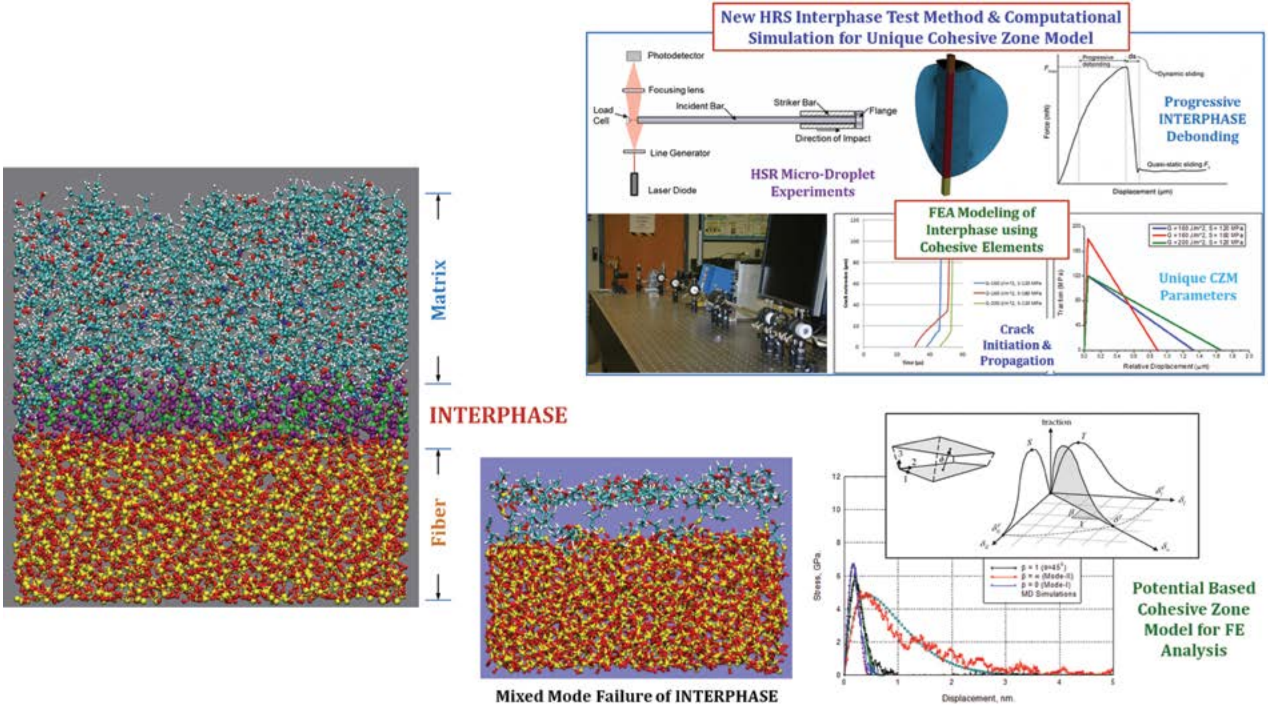


Figure 9: *Methodology for Composites Fiber-Matrix Interphase by Design.*

Designing Epoxy Networks Through Molecular Simulations

Professor Cameron F. Abrams *Drexel University*	**Professor Giuseppe Palmese** *Drexel University*	**Dr. Jan Andzelm** *Army Research Laboratory*
Dr. Timothy Sirk *Army Research Laboratory*	**Dr. Chang Woon Jang** *Postdoctoral Fellow, Drexel University*	**Mr. Majid Sharifi** *Graduate Student, Drexel University*

We developed a multi-step crosslinking algorithm [1-3] for designing epoxy thermoset polymers and compared this algorithm with one-step Monte Carlo crosslinking method. We found that most material properties are insensitive to the method choice, but the one-step crosslinking method produced more ramified networks as compared to those produced by the more gradual multi-step approach. All-atom molecular dynamics simulations reproduced two types of engineered thermoset polymers cured by 1) Reactive Encapsulation of Solvent (RES) [1] and 2) Partially Reacted Substructure (PRS) [3] curing protocols as shown in Figure 10. Simulations were verified against experimental results in terms of thermal, structural, and mechanical properties. The PRS influence on tetra-functional epoxy/Jeffamine diamine/Jeffamine monoamine polymers is being further investigated to explain the atomic-scale origins the toughness enhancement. The findings in these studies will provide further guidance in the use of control over optimized properties of epoxy matrices in composite materials.

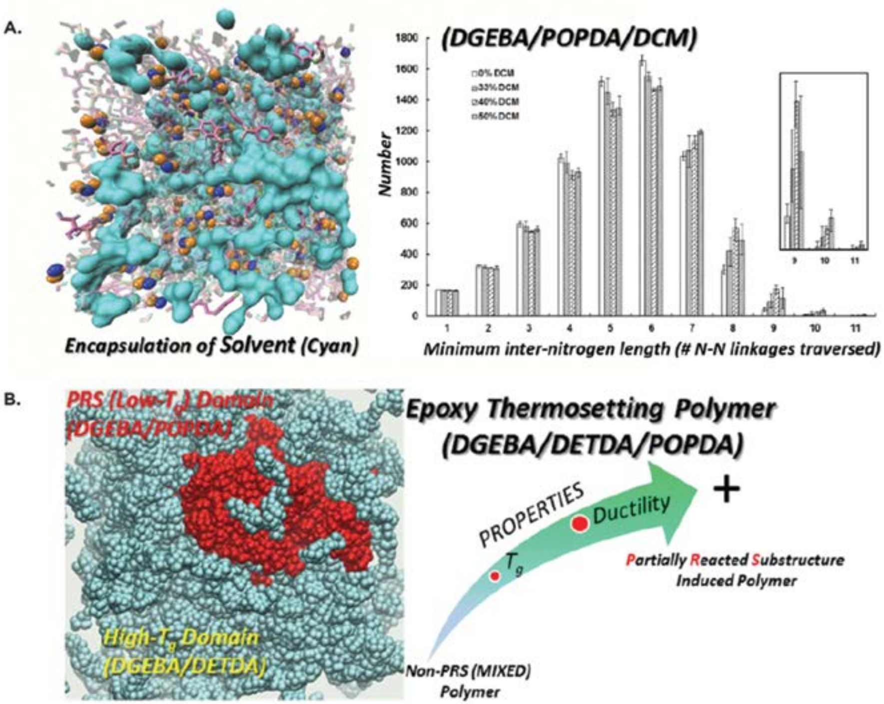


Figure 10: *Snapshots from representative all-atom MD simulations of two engineered thermoset polymers cured by (a) Encapsulation of solvent (RES) and (b) Partially Reacted Substructure (PRS) protocols. Right-hand panel in (a) shows the distribution in inter-nitrogen path lengths and how this distribution shifts to longer path lengths as the amount of inert solvent present during curing increases.*

References:

1. C Jang, M Sharifi, GR Palmese, CF Abrams, Polymer, 2014, 55 (16), 3859-3868.

2. C Jang, TW Sirk, JW Andzelm, CF Abrams, Macromolecular Theory and Simulations, 2015, 24 (3), 260-270.

3. C Jang, M Sharifi, GR Palmese, CF Abrams, Polymer, 2015. (Under Review)

RESEARCHER HIGHLIGHT: SUBRAMANI ‘MANI’ SOCKALINGAM

Hailing from India, Mani currently works with the MEDE program as a Graduate PhD candidate in Mechanical Engineering at the University of Delaware co-advised by Dr. John W. Gillespie Jr. and Dr. Michael Keefe.

What are your current activities with MEDE?
My activities within MEDE are in both Composites and Polymers groups. In composites, I work on developing high strain-rate fiber-matrix interfacial traction separation laws at the micromechanical length scale in order to establish a Materials-by-Design framework. In polymers, I work on developing micron length scale modeling and experiments to understand the fundamental high performance polymer fiber behavior during ballistic impact. All these activities involve collaborations with ARL and other MEDE consortium members.

Tell us about your interests and goals.
I enjoy biking, hiking, traveling and volunteering. I volunteered at CARE7 crisis response team, in Tempe, AZ and also volunteered as a tutor at Arredondo Elementary, Tempe, AZ through All Star Kids Tutoring. One of my goals in the near future is to bike a century (100 miles) in a day and not be injured!

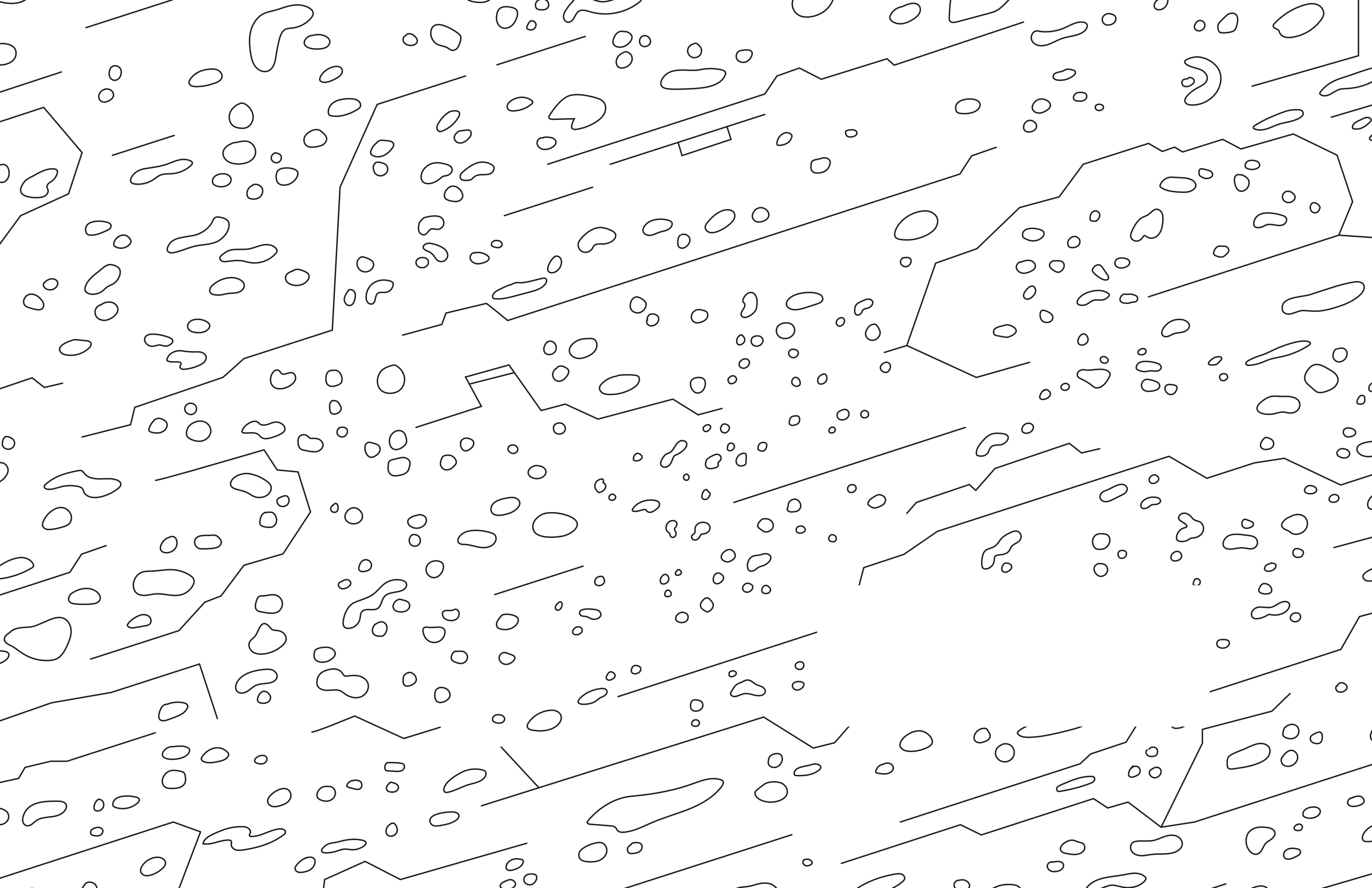
What would you consider some of your biggest accomplishments?
I’ve been fortunate enough to have a lot of memorable moments thus far in my career. A few standouts are: receiving a Certificate of Merit during my undergraduate studies from the former President of India Dr. A.P.J Abdul Kalam, my MS thesis defense and graduation at the University of Cincinnati, working with Ford Motor Company on structural safety analysis of next generation Ford vehicles, receiving the American Society for Composites (ASC) PhD scholarship in 2014 at the ASC Conference in San Diego, and receiving the R.L. McCullough Scholar Award in 2015 at the Center for Composite Materials (CCM), University of Delaware.

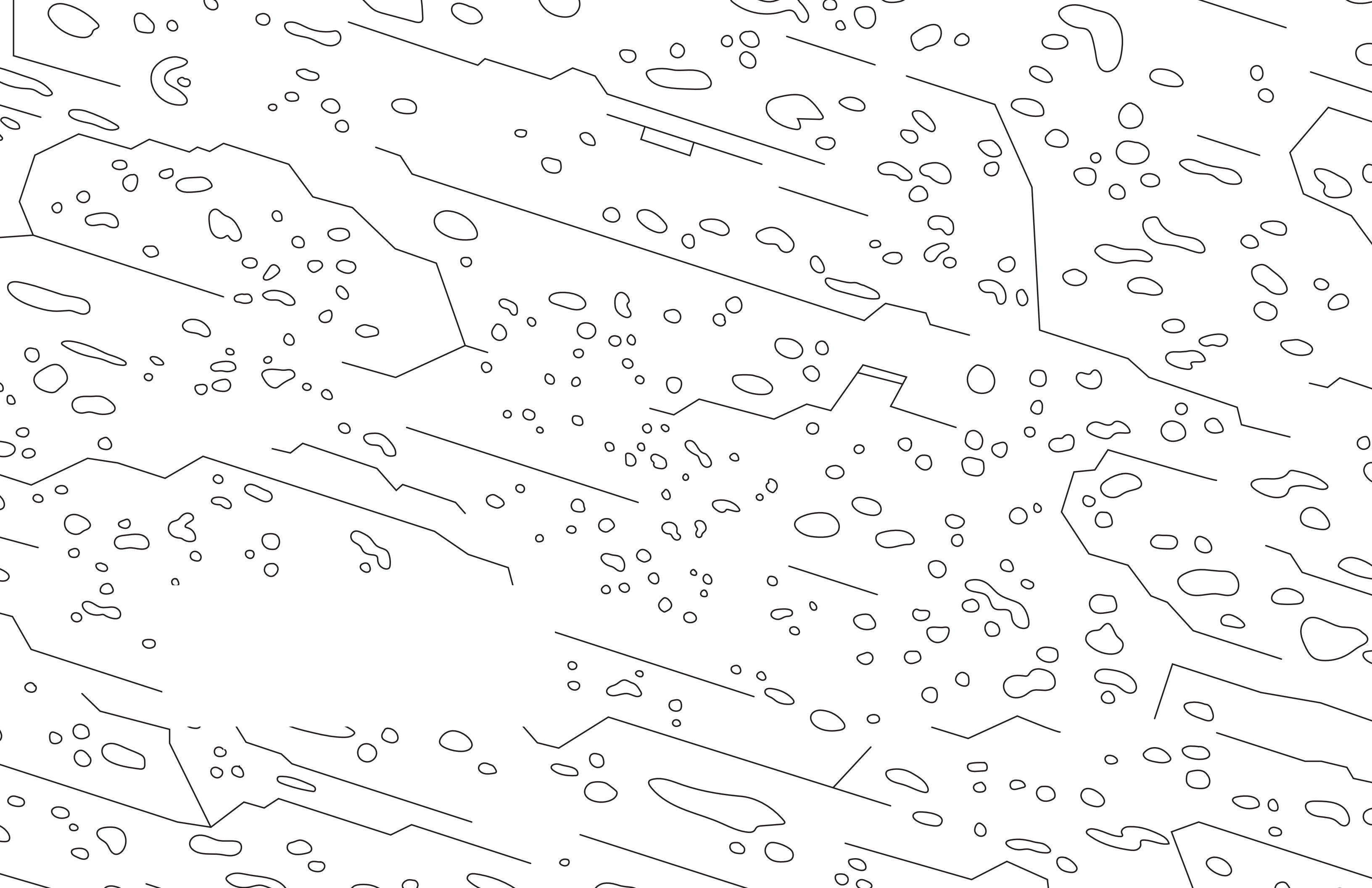
Who are your biggest influences in both your personal and professional life?
Professionally - My advisors during my masters, PhD and supervisors during my industry experience in designing body and vehicle armors and automotive crashworthiness as well as my fellow team members and students. They all help me to continuously learn new things and move forward in terms of research, acquiring new knowledge and developing communication skills. It’s because of them that I aspire to become a faculty in the near future to conduct research, teach and inspire the next generation students.

Personally - My family and all my friends that are always there for me, especially during tough times.

> **The collaboration aspect of the MEDE program allows us to leverage the expertise of ARL and consortium members. As a student, the program gives me an opportunity to interact with and learn from experts in different areas which otherwise would not have been possible.**

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

Dr. Tom Arsenlis, LLNL

Prof. Kaushik Bhattacharya, Caltech

Prof. Bob Cammarata, JHU

Prof. Jaafar El-Awady, JHU

Prof. Michael Falk, JHU

Prof. Yogendra Gupta, WSU

Prof. Kevin Hemker, JHU

Prof. Todd Hufnagel, JHU

Prof. Jamie Kimberley, NMT

Prof. Dennis Kochmann, Caltech

Prof. Michael Ortiz, Caltech

Prof. Guruswami Ravichandran, Caltech

Prof. K.T. Ramesh, JHU

Prof. Tim Weihs, JHU

Prof. Justin Wilkerson, UTSA

ARL COLLABORATORS

Mr. Brady Butler

Dr. Daniel Casem

Dr. Vince Hammond

Dr. Tyrone Jones

Dr. Laszlo Kecskes

Dr. Jeffrey Lloyd

Dr. Heidi Maupin

Dr. Tomoko Sano

Dr. Brian Schuster

Dr. Mark Tschopp

Dr. N. Scott Weingarten

Dr. Cyril Williams

CONSORTIUM RESEARCH TASKS

- In situ x-ray diffraction and imaging during dynamic loading (Hufnagel, JHU)
- High rate DTEM mechanical testing (Weihs, JHU)
- High strain-rate characterization of magnesium and its alloys (Ramesh, JHU)
- TEM characterization of dislocation structures in Mg (Hemker, JHU)
- Atomistic and discrete dislocation dynamics modeling of mechanical twinning and plasticity (El-Awady, JHU)
- Thermo-mechanical processing of Mg alloys (Weihs, JHU)
- MD of nucleation and motion of defects (Falk and Cammarata, JHU)
- Coarse-grained DFT (Bhattacharya, Caltech)
- Hot quasi-continuum methods (Ortiz, Caltech)
- Thermo-mechanical behavior of magnesium alloys (Ravichandran, Caltech)
- Continuum models for plasticity-twinning interactions in magnesium (Kochmann, Caltech)
- Deformation mechanisms in shocked pure and alloyed Mg single crystals (Gupta, Washington State)
- Dynamic microscale tensile testing of magnesium (Kimberley, NMT)
- DD FEM (predict twinning using FEM) (Arsenlis, LLNL)
- A simple constitutive framework for anisotropic dynamic ductile failure (Wilkerson, UTSA)

Dynamic Mechanisms in Magnesium

Professor Dennis Kochmann
California Institute of Technology

Dr. Jeffrey Lloyd
Army Research Laboratory

Dr. Owen Kingstedt
California Institute of Technology

We have developed a new computational methodology that enables us to describe, understand, and predict the intricate deformation and failure mechanisms in magnesium under high-rate dynamic loading conditions. Modeling magnesium poses particular challenges due to the competition between dislocation plasticity and deformation twinning, two quite distinct mechanisms that affect the material's performance, e.g., its strength, ductility, or toughness. The new modeling strategy aims at finding a compromise between a detailed, accurate description of the underlying microstructural processes and an efficient computational approach that is applicable at the macroscale, i.e., at the device level, rather than at microstructural length and time scales. The resulting model is rate-sensitive (i.e., it captures the dependence on loading rate) and has been validated by comparison with benchmark experiments. In addition, its variational structure equips the model with superior efficiency – compared to many competing (explicit) models, the time step used in (implicit) calculations can be significantly larger, thereby enabling the simulation of longer processes through a considerable reduction of the required computing time. By modeling the deformation response of polycrystalline magnesium (with texture details obtained from experiments), simulations predict the distribution of slip and twinning throughout the sample during loading and also hint at hot spots for failure. The model also predicts the temperature rise during loading, which is directly comparable to temperature measurements from high-rate experiments (such as those performed by the group of Caltech collaborator Prof. Ravichandran) and therefore also serves to inform and validate the model.

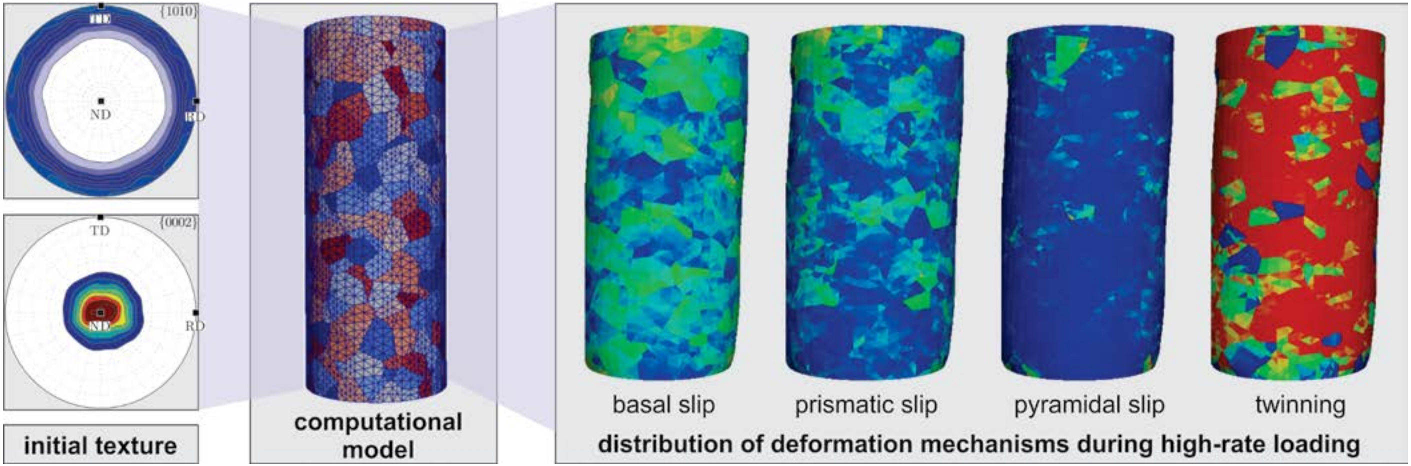


Figure 11: *By incorporating experimental information about the initial texture (here, for a cold-rolled sample), a polycrystalline sample is represented by a finite element model (containing about 1000 grains), so that simulations of high-rate compression reveal the slip and twinning contributions to the observed inelastic deformation of the sample.*

X-ray Experiments Explore the High Strain-Rate World of Magnesium

Professor Todd Hufnagel
Johns Hopkins University

Dr. Daniel Casem
Army Research Laboratory

Our research is providing an invaluable look at the processes occurring at crystalline scales in real time and will allow for validation of atomistic and crystalline-level models that are being developed within the ARL Enterprise for Multiscale Research in Materials (EMRM), and the Materials for Extreme Dynamic Environments Collaborative Research Alliance (MEDE CRA).

The experiments rely on x-rays produced from the Cornell High Energy Synchrotron Source (CHESS), and a fast-pixel array x-ray detector, to study the crystal plasticity of magnesium at high strain rates. These experiments achieved temporal resolution on the microsecond and sub-microsecond scales during high-strain-rate Kolsky bar experiments.

CHESS provides users with high-intensity, high-energy x-rays for research in physics, chemistry, biology, and environmental and materials sciences. A synchrotron is an extremely powerful source of x-rays.

We are analyzing the data to see whether they support current theories about the high-strain-rate behavior of magnesium. Going forward, we are designing new experiments that will provide even more detailed information about how a wide range of materials deform and fracture under high-rate loading.

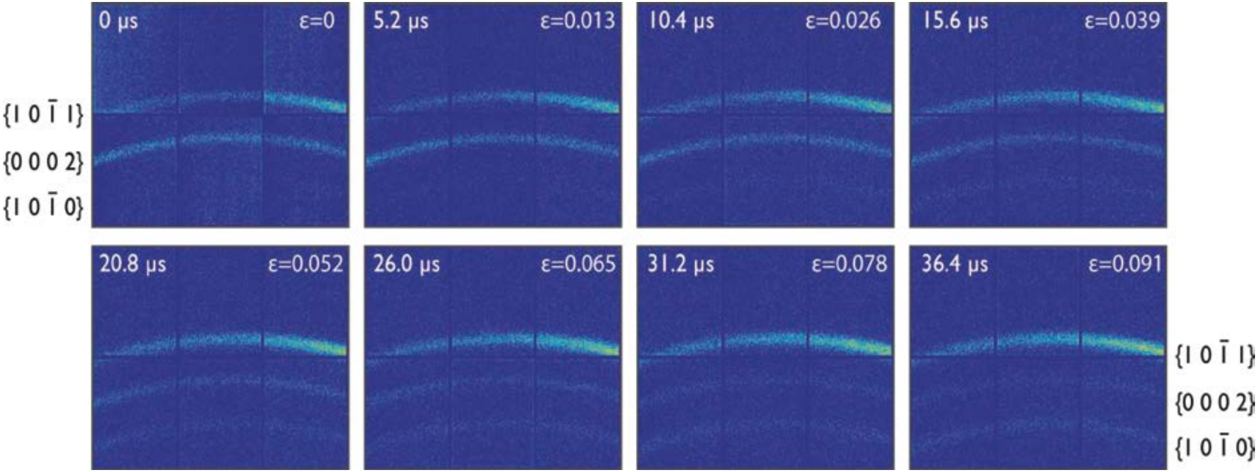


Figure 12: *Diffraction patterns recording during high-strain-rate compression of Mg AZ31B recorded at CHESS on a pixel array detector. The disappearance of the {0002} diffraction line and the simultaneous strengthening of the {1 0 1̄ 0} line are due to extension twinning.*

RESEARCHER HIGHLIGHT: CALEB HUSTEDT

Caleb is a graduate student at Johns Hopkins University who originally began working on the femtosecond laser 3D serial sectioning project, but has since switched to doing in situ x-ray diffraction.

What is/are the most memorable moment(s) to date in your professional career?
Performing my first experiments at the synchrotron and getting good data. Finishing my undergraduate career and subsequently being accepted to graduate school here at Hopkins. Presenting at various conferences such as MRS, SEM, or MACH.

What are some of your goals?
Two goals that I'd like to achieve by the end of the 2015 calendar year are to publish data on deformation twinning in magnesium and to sleep train my youngest child.

Tell us about your interests.
Within the MEDE program, my interests lie with lightweight metals, including magnesium. Additionally, I'm interested in x-ray diffraction using synchrotron radiation and electron microscopy.

Outside of work, I enjoy spending time with my two children doing various family-friendly activities around Baltimore - the zoo, the MD Science Center and the B&O museum are some of our favorite spots. I also enjoy playing both indoor and outdoor soccer.

Who are your biggest influences in both your personal and professional life?
Personally - My wife and children. They provide motivation and support for everything I do.

Professionally - Both my graduate and undergraduate advisors, Todd Hufnagel and Robert Davis respectively. They have shaped what I have worked on and assisted me in growing professionally.

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. Kadir Aslan, Morgan State

Prof. Wayne Chen, Purdue

Prof. Joe Deitzel, Delaware

Prof. Jack Gillespie, Delaware

Prof. Vicky Nguyen, JHU

Prof. Giuseppe Palmese, Drexel

Prof. Mark Robbins, JHU

ARL COLLABORATORS

Dr. Jan Andzelm

Dr. Travis Bogetti

Dr. Tanya Chantawansri

Dr. Joseph Lenhart

Dr. Bryan Love

Dr. James Snyder

Dr. Tusit Weerasooriya

Dr. Nicole Zander

CONSORTIUM RESEARCH TASKS

- Characterization of meso/nanoscale domains in UHMWPE fibers (Gillespie and Deitzel, Delaware)
- Linking to the fibers industry (Gillespie, Delaware)
- High-rate behavior of UHMWPE (Chen, Purdue)
- Micromechanical model of the rate-dependent and temperature-dependent of highly oriented polyethylene fibers (Nguyen, JHU)
- Potentials for modeling polymer deformation (Robbins, JHU)
- Bulk porosity of various polymer samples of UHMWPE (Aslan, Morgan State)

Dynamic Mechanical Behavior of Single Ballistic Fibers

Professor Wayne Chen
Purdue University

Professor Joseph Deitzel
University of Delaware

Dr. Daniel Casem
Army Research Laboratory

In this research effort, the mechanical response of single filaments of high-performance fibers, including Spectra®100d and 13d have been determined under uniaxial tension, tension/shear, and transverse compression loading conditions with loading rates varying from quasi-static to dynamic. Single fibers are subjected to various known levels of both torsional shear strain and axial tensile stress to determine the effects of combined loading on the tensile strength. Axial tension experiments are performed on pre-twisted fibers using a miniature tension Kolsky bar and MTS servo-hydraulic system. The resulting torque generated by fibers loaded to specific degrees of shear strain is determined using an in-house developed torque sensing technique. Compilation of the two stress states has generated a biaxial failure surface criterion yielding the residual tensile strength of single fibers when subjected to a specific level of shear stress. To study the fiber response under transverse compression, we use an improved method for fiber transverse compression developed previously. Two fiber specimens are laid parallel and compressed between two tool steel platens to obtain the nominal stress–strain curves under quasi-static loading. To evaluate the rate effects on the transverse behavior, high-rate transverse compression experiments are performed at ARL using a miniature Kolsky bar.

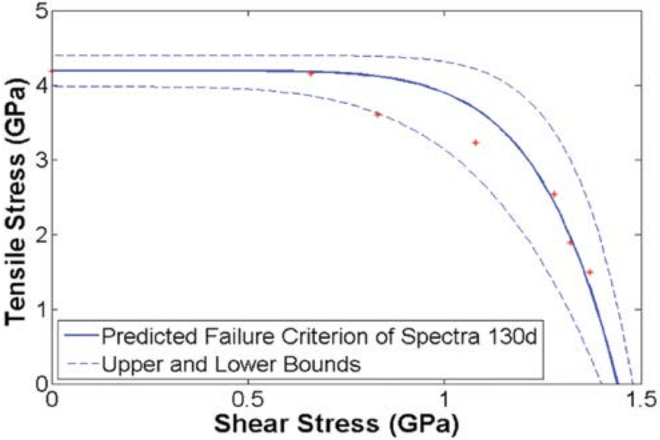


Figure 13: *Bi-axial failure surface of Spectra® 130d.*

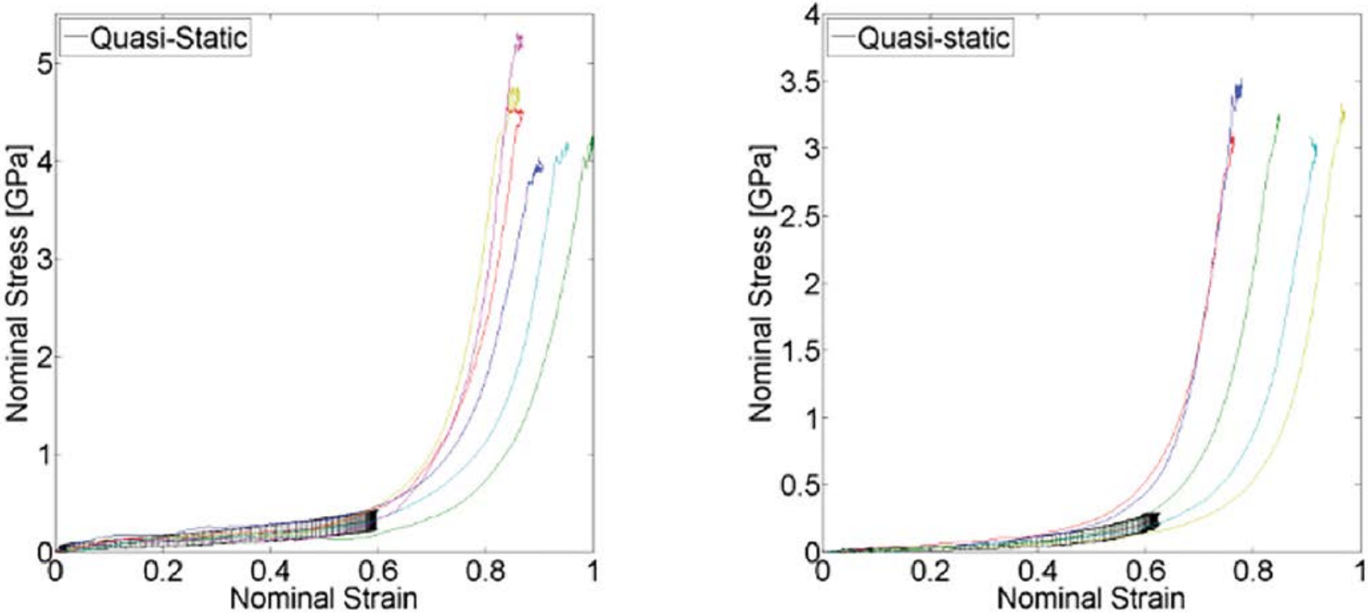


Figure 14: *Dynamic transverse compressive response of Kevlar (left) and Dyneema (right) single fibers (the data below 0.6 strain with error bands are quasi-static results).*

Atomistic modeling of the Ultra-High Molecular Weight Polyethylene (UHMWPE) system

Professor Mark Robbins
Johns Hopkins University

Dr. Jan Andzelm
Army Research Laboratory

Dr. Tanya Chantawansri
Army Research Laboratory

Today's soldiers rely on polymers as part of their protective systems. However, 20 to 30 years from now, our soldiers will need protective systems that can stand up against tougher threats that are certain to be developed. We have collaborated to elucidate mechanisms of deformation and failure in polyethylene using atomistic simulations and coarse-graining methods. [1-3] Key to modeling this system was the development of reactive potentials to be used in atomistic modeling of the Ultra-High Molecular Weight Polyethylene (UHMWPE) system.

We have successfully accomplished this by using accurate quantum mechanical data to parameterize an atomistic potential, referred to as the "AIREBO-M" potential, that has been verified to be both computationally fast and accurate (Figure 15). It captures the crystal structure and shock response of polyethylene to pressures of more than 40GPa and accurately describes bond-breaking.

Methods to "coarse-grain" and "back map" to the atomistic level have also been developed under this collaboration. This will allow computations to further bridge time and length scales that are currently beyond the reach of atomistic level modeling. In turn, these methods will feed higher level micro-mechanical models, such as those being developed in another portion of the program by Dr. Vicky Nguyen of Johns Hopkins University.

Critical to developing computational models is the ability to synthesize and characterize well-defined model systems. This data provides valuable input and validation to the computational models. We joined with the ARL's Center for Advanced Polymer Processing to develop computational methods to model polyethylene fibrils being pulled at high rates (Figure 16). This work is providing great insight into how small scale behavior determines macroscopic response. For example, recent simulations show that atomic scale defects can explain the decreased strength of experimental fibers compared to ideal theoretical predictions.

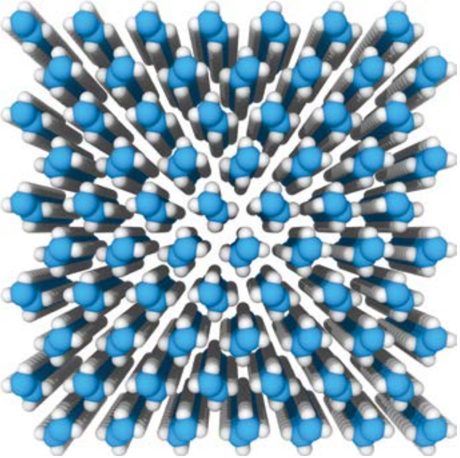


Figure 15: *The new AIREBO-M Potentials were validated against a pressure-volume isotherm at T=533K for polyethylene crystals. The AIREBO-M potentials showed nearly perfect agreement with REAXFF calculations and experimental data. However the AIREBO-M potentials were much more computationally efficient than REAXFF calculations, and provided a more accurate description of bond breaking.*

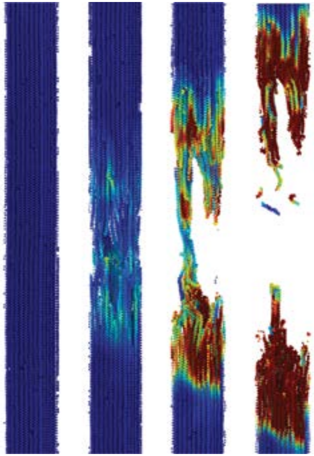


Figure 16: *AIREBO-M simulations of tensile failure of a polyethylene fiber show that the final fracture (right) is due to slip of chain ends, reducing the fiber strength by a factor of 4 relative to an ideal crystal. AIREBO-M is also being used to study compressive impact [3].*

References:

1. Computational Modeling of Polyethylene at ARL, Tanya Chantawansri, In-Chul Yeh, Timothy Sirk, Joshua Moore, John Brennan, Jan Andzelm, Mach Conference, Annapolis MD, April 9-11, 2014.

2. AIREBO-M: A Reactive Model for Hydrocarbons at Extreme Pressures, Thomas C. O'Connor, Jan W. Andzelm, Mark O. Robbins, The Journal of Chemical Physics 142, 024903 (2015); doi: 10.1063/1.4905549

3. Atomic-scale investigation of shock front propagation through crystalline and amorphous polyethylene, Thomas C. O'Connor, Vikram Jadhao, Mark O.Robbins, Robert Elder, Timothy Sirk, Tanya Chantawansri, Jan Andzelm, Mach Conference, Annapolis MD, April 8-10, 2015.

RESEARCHER HIGHLIGHT: PRESTON MCDANIEL

Preston is a graduate student working at the University of Delaware within the Center for Composite Materials. He currently works on the characterization of the meso/nanostructure in UHMWPE fibers. He is also involved in studying the meso/nanoscale energy dissipative mechanisms in the UHMWPE fibers.

How did you get involved with the MEDE program?
When I started graduate school, I chose to work at the UD Center for Composite Materials. I spoke with my advisors, Dr. Jack Gillespie and Dr. Joe Deitzel about funded projects that I might be involved with. Based on my undergraduate degree in Polymer Science from the University of Southern Mississippi, we decided that my knowledge and interests made me a good fit for the MEDE Polymers program.

Tell us about your interests.
Professionally, I am interested in new and novel applications of polymers and polymer composites. I enjoy studying the microstructure of polymer materials and understanding the role these features play in the macroscopic mechanical response of materials.

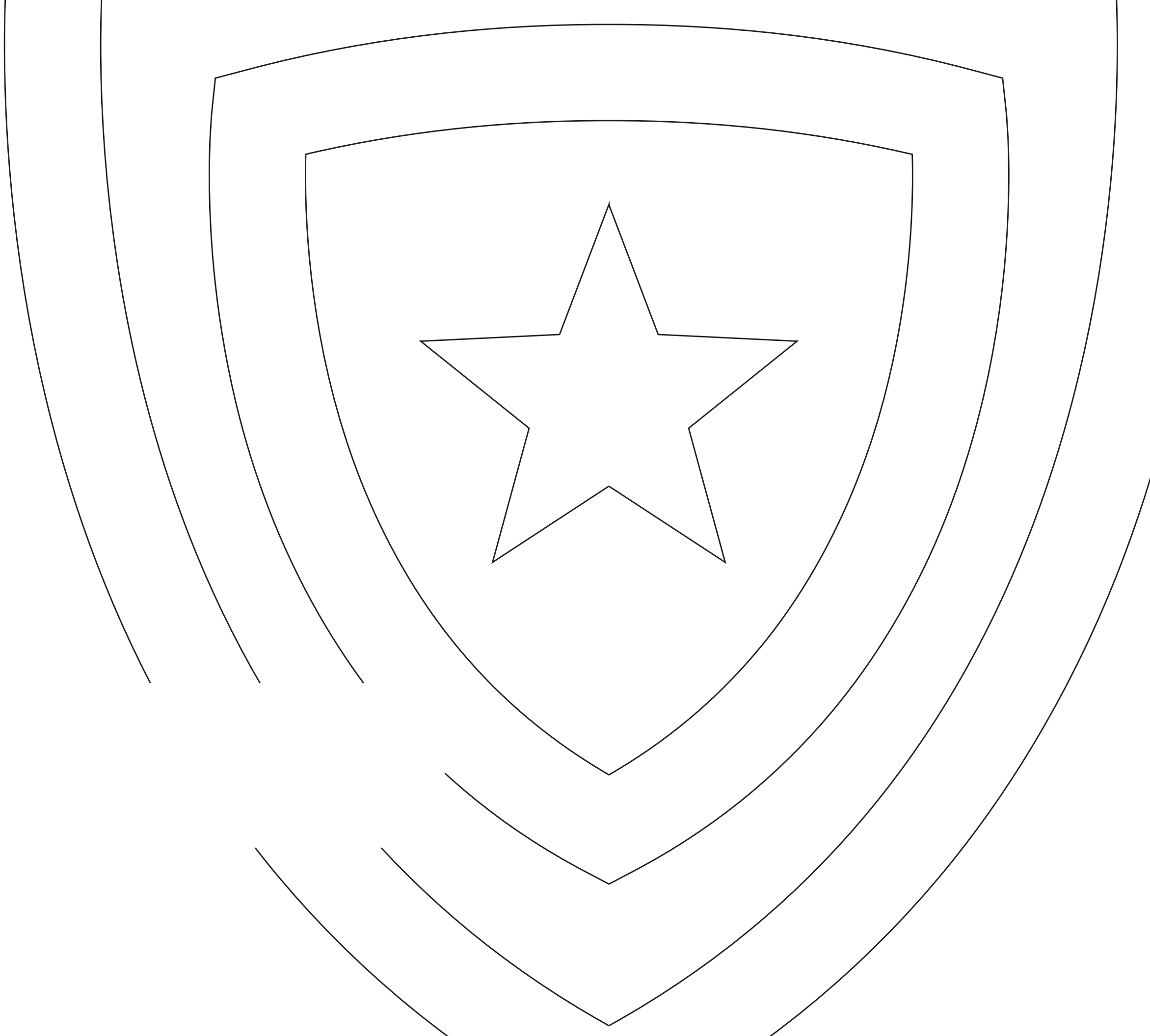
In my personal life, I love sports. Coming from the Houston area, I am a die-hard fan of all Houston sports teams (the Astros made me proud this year). I also enjoy outdoor activities. I am blessed to have a great group of friends that love to go camping and hiking, and I am always looking for an opportunity to do either of these things.

What are some goals you have for the future?
I am hoping to finish my Ph.D. by the end of 2016. After that, I would like to either work in industrial R&D or perhaps in a national lab. My wife and I would also like to adopt a child, as we are both very passionate about orphan care.

Who is your biggest influence professionally and why?
As cliché as it sounds, I have to say that my advisors Dr. Gillespie and Dr. Deitzel have both played a huge role in my development as a researcher. They both hold me to a high standard and constantly encourage me to push my boundaries. Much of what I learn from them also goes so far beyond just the interactions concerning my research. Observing the way they approach complex problems and handle difficult situations has been key to my growth.

> **The MEDE program has provided an excellent platform for me to collaborate with researchers from multiple universities and the Army Research Lab. The experience I have gained from these collaborations has been invaluable, and I have learned so much through these interactions.**

The CMEDE shield showcases the integration and collaboration found within the MEDE program.



INTEGRATIVE AND COLLABORATIVE TOOLS


Prof. K.T. Ramesh


Prof. Lori Graham-Brady


Prof. Tamas Budavari


Dr. Betsy Rice


Dr. Richard Becker

SOME CONSORTIUM PRINCIPAL INVESTIGATORS

Prof. Kaushik Bhattacharya, Caltech

Prof. Tamas Budavari, JHU

Prof. Lori Graham-Brady, JHU

Prof. Michael Kirby, University of Utah

Prof. K.T. Ramesh, JHU

SOME ARL COLLABORATORS

Dr. Richard Becker

Dr. Travis Bogetti

Mr. Brian Leavy

Dr. William Mattson

Dr. Danny O'Brien

Dr. Betsy Rice

CONSORTIUM RESEARCH TASKS

- Integrated Models for Magnesium Alloys (Bhattacharya, Caltech and Ramesh, JHU)
- Probabilistic Modeling and Uncertainty Quantification for Computational Models of Composites (Graham-Brady, JHU)
- Data-Intensive Science for Materials in Extreme Dynamic Environments (Budavari, JHU)

Integrated models for magnesium alloys

Professor Kaushik Bhattacharya
California Institute of Technology

Professor K.T. Ramesh
Johns Hopkins University

Dr. Richard Becker
Army Research Laboratory

Goal: To develop an integrated model of the deformation and failure mechanisms of Mg alloys that can be used as a bridge between the fine-scale models of unit processes and canonical models.

Research strategy: For each deformation or failure mechanism that is a part of the canonical model, we build an integrated model that is rich enough to describe the mechanism in the complexity relevant for Mg alloys in extreme dynamic environments and has the room to incorporate information from smaller scale models. Our strategy is to first start with one mechanism – tentatively spallation or localization, develop an integrated model for this, and verify and validate it. Once this strategy is demonstrated on one mechanism, it will be extended to other mechanisms in future years.

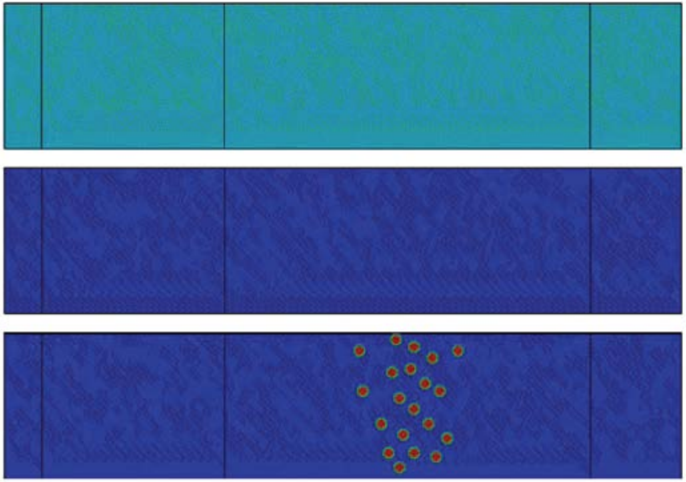


Figure 17: Modeling the spallation of magnesium.

Probabilistic Modeling and Uncertainty Quantification for computational models of composites

Professor Lori Graham-Brady
Johns Hopkins University

Professor Michael Kirby
University of Utah

Goal: The long-term goal of this project is to develop a framework for uncertainty quantification (UQ) and/or probabilistic modeling of materials for armor applications. Because composites can be an ideal case study for materials with inherent uncertainties, we select composites as the test bed for developing UQ models for armor.

Research strategy: Assembling a joint team from the MEDE and MSME CRAs and ARL that that addresses probabilistic modeling and UQ for mechanics and upscaling models for composites, a multi-scale model for composites that incorporates uncertainties will be developed.

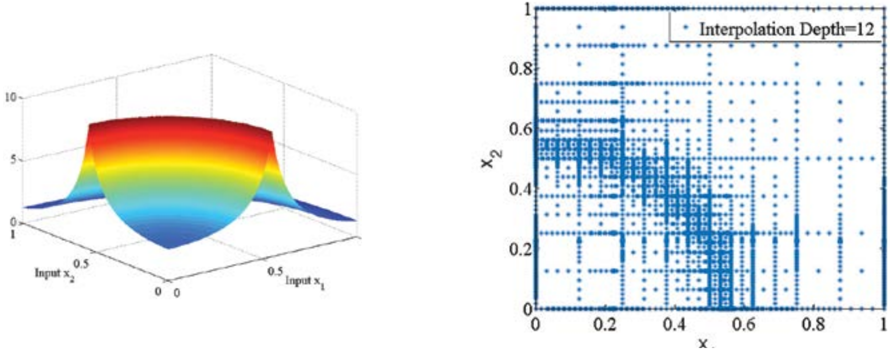


Figure 18: *Adaptive sparse grid sampling in two-dimensional space, capturing a discontinuous response surface with minimal number of model evaluations. This is expected to be particularly important for composite behavior such as debonding which will lead to such discontinuities.*

Data-Intensive Science for MEDE

Professor Tamas Budavari

Johns Hopkins University

Goal: An organically integrated data science effort in the Materials in Extreme Dynamic Environments (MEDE) project to facilitate seamless connections among the experimental, processing and modeling researchers. The foundation of such an effort would be a novel infrastructure that can dynamically federate the separate components.

Research Strategy: Protocol, interface and database designs patterns are readily available with flexible implementations, e.g., CasJobs (online at skyserver.sdss.org/casjobs). The Institute for Data Intensive Engineering and Science (IDIES) at JHU is already spearheading SciServer – a large Data Infrastructure Building Blocks (DIBBs) project funded by NSF - which provides turnkey solutions for a number of common problems, for example, single sign on authentication or file sharing. The SciDrive (www.scidrive.org) – one of the key SciServer initiatives – presents a convenient framework for safely storing and sharing files; similar to the Dropbox and Box.net services. SciDrive, however, comes with the added benefit of a plugin architecture that can be customized for different scientific domains: it can automatically act on specific file formats. We will use and adapt concepts and technologies originally developed for the astronomy community to the advancement of this materials-by-design program.

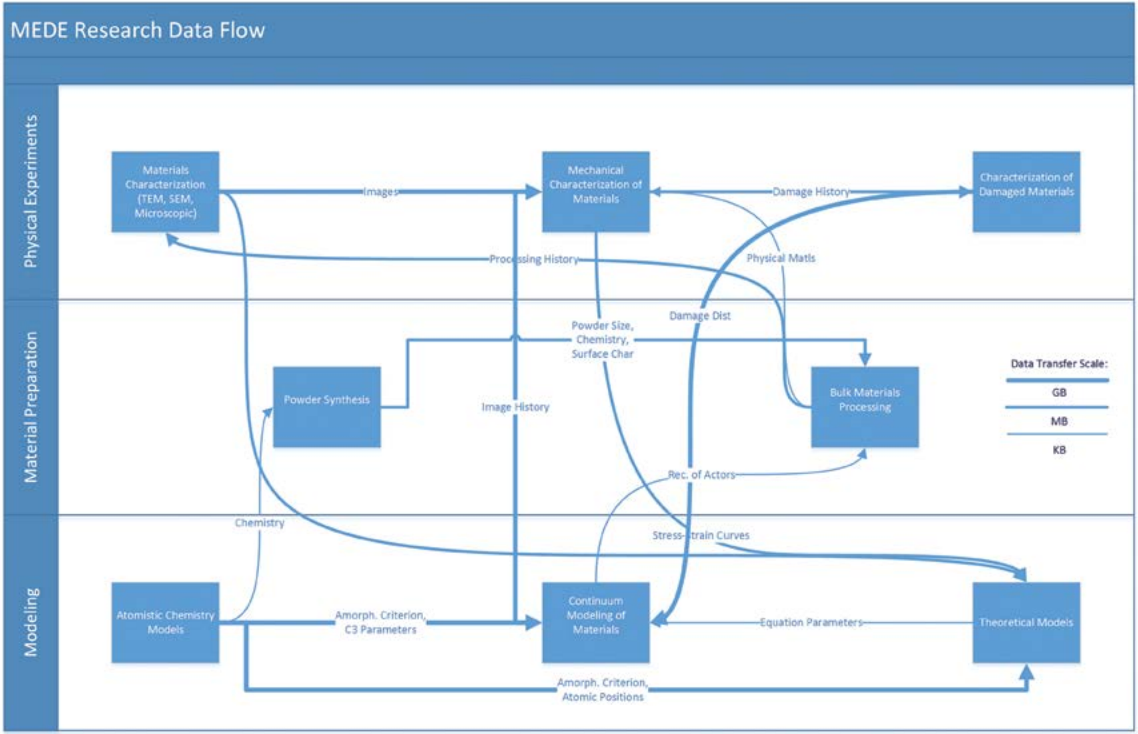


Figure 19: *An example of data flow within the Ceramics CMRG.*

ADDITIONAL COLLABORATIVE ACTIVITIES

ARL Open Campus

Another way ARL and consortium members collaborate is through 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 encourage groundbreaking advances in basic and applied research areas of relevance to the Army.

Defence Science and Technology Laboratory (DSTL)

On September 30, 2015, Professor KT Ramesh, Director of CMEDE, and Dr. John Beatty, Senior Materials Researcher at the Army Research Laboratory, led an eleven person US delegation to meet with scientists in the United Kingdom (UK) to discuss protection materials research. The meeting was hosted by the Defence Science and Technology Laboratory (DSTL) and held at the UK Defence Academy in Shrivenham.

The meeting had over 50 attendees and included presentations focused on materials research under dynamic, high strain-rate conditions similar to those found in a blast or ballistic environment. The results of this research will assist in developing improved protection materials for soldiers and vehicles. A particular focus was on sharing experimental, modeling and processing research of ceramic materials currently being conducted in conjunction with the Center for Materials in Extreme Dynamic Environments (CMEDE) located at Johns Hopkins University.

Additional continuing activities between the United States and the United Kingdom are being explored. This event demonstrates the continued commitment towards international engagements by the CMEDE, Army Research Laboratory, and DSTL.

MEDE Fall Meeting

The CMEDE Fall Meeting is an annual event that brings members of the MEDE CRA and researchers from the Army Research Laboratory together for two days of collaborative activities and discussion. In 2015, special guests from the United Kingdom's Defence Science and Technology Laboratory, Army Research Office, and Office of Naval Research participated in the meeting as well.

Mach Conference

The Mach Conference is an annual 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.

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 – Two day courses co-sponsored by the Hopkins Extreme Materials Institute that are taught by recognized experts in the area of materials in extreme dynamic environments. Attendees include representatives from academia, government and industry.
- 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.
- MEDE Undergraduate Internships – Paid summer internships for students at the MEDE Consortium locations that assist in developing research skills for undergraduate students.

Collaborative

- Extreme Science Internships (ESI) – Led by Dr. Alvin Kennedy, 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.
- Extreme Science Scholars (ESS) – The ESS program supports Morgan State University students with funding provided by the Army Research Laboratory based on special interest by the Maryland Congressional delegation. Morgan State University ESS program students are at the graduate and/or undergraduate level and pursuing a math, science, engineering or technology degree. The ESS program is an expansion of the current Extreme Science Internship (ESI) program.
- HEMI/MICA Extreme Arts Program – The HEMI/MICA Extreme Arts Program is a new initiative that brings faculty and students from both institutions 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 dialog will create a stronger community through a shared sense of curiosity and exploration. CMEDE is a significant participant in this program.

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1. *Dr. Charles Anderson, SwRI*
2. *Dr. Gerald Kerley, Kerley Technical Services*
3. *Dr. Lalit Chhabildas, Air Force Research Laboratory*
4. *JHU/MSU ESI signing ceremony*
5. *2015 Extreme Science Scholars are presented certificates from program sponsors*
6. *HEMI/MICA Extreme Arts Program Intern Samantha French*

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)

Center of Excellence on Intergrated Materials Modeling

US Advanced Ceramics Association (USACA)

Lightweight Innovations for Tomorrow (LIFT)

Ceramics, Composite and Optical Materials Center (CCOMC)

FACILITIES AND EQUIPMENT

The facilities and equipment within the MEDE CRA provide state-of-art capabilities to support experimental, computational and processing research activities. A small sampling of the facilities and equipment found at MEDE consortium locations is included in this section.

FACILITIES

Malone Hall – Opened in July of 2014, Malone Hall at Johns Hopkins University provides over 20,000 square feet of administrative, collaborative meeting, and laboratory space for CMEDE. With its wireless network and infrastructure, Malone Hall hosts monthly CMRG meetings, science advisory boards, seminars and short courses. Additionally, in support of the ARL Open Campus Initiative, dedicated office space for MEDE consortium members and ARL researchers is available and is utilized regularly.

Maryland Advanced Research Computing Center (MARCC) – MARCC is a shared computing facility located on the Bayview Campus of Johns Hopkins University. The main cluster at MARCC has over 19,000 cores and a combined theoretical performance of over 900 TFLOPs. It also features two types of storage: 2 PB Lustre (Terascala) and 15 PB ZFS/Linux.

Center for Composite Materials (CCM) – Located at the University of Delaware, CCM 52,000-square-foot, state-of-the-art, facilities consist of the Manufacturing Sciences Laboratory and the Applications and Technology Transfer Laboratory. CCM develops models and simulations in a “virtual manufacturing” environment for process optimization and tool design, leading to improved quality, affordability, and innovative new composite manufacturing processes.

Ceramic, Composite and Optical Materials Center (CCOMC) – Rutgers University is the home of the CCOMC which provides state-of-the-art equipment for ceramic powder synthesis, characterization and processing, ranging from laboratory to pilot scale capacities. CCOMC provides a facility that can be used in the seamless, synergistic and cooperative research collaboration for any program.

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1. Malone Hall Exterior
2. Malone Hall Interior
3. Ceramic, Composite and Optical Materials Center (CCOMC)
4. Maryland Advanced Research Computing Center (MARCC)

EQUIPMENT

Select Equipment at Multiple MEDE Consortium Institutions

Kolsky (Split-Hopkinson) Bars – Kolsky bars are used to test the dynamic stress-strain response of a particular material. Tension and compression Kolsky bars in combination with high-speed imaging is extensively in the characterization of materials. MEDE institutions with Kolsky bars include: Johns Hopkins, Caltech, New Mexico Tech, and Purdue.

Scanning Electron Microscopes (SEM) – SEMs produce high-resolution, dimensional images showcasing topographical, morphological and compositional information of different materials. A 3-dimensional SEM is in development at Johns Hopkins while 2-dimensional SEMs are used by Caltech, Delaware and Washington State. The 3-dimensional SEM will use focused ion beam (FIB) milling together with orientation imaging by electron backscatter diffraction (EBSD) to perform serial sectioning experiments.

Transmission Electron Microscopes (TEM) – TEMs are used to produce high-resolution, two-dimensional images at the atomic level, finding insight to their structure as they are placed under stress. TEMs are primarily used by Johns Hopkins, Caltech, and Delaware.

Dynamic Transmission Electron Microscope (DTEM) – The goal of the DTEM is to perform in situ imaging of material deformation during rapid loading. This new, mechanical testing technique will identify dislocation and twin motion as a function of strain-rates in the range of 10^2 to 10^5 s^{-1}. The DTEM project is being led by Johns Hopkins uses key facilitites at Lawrence Livermore National Laboratory.

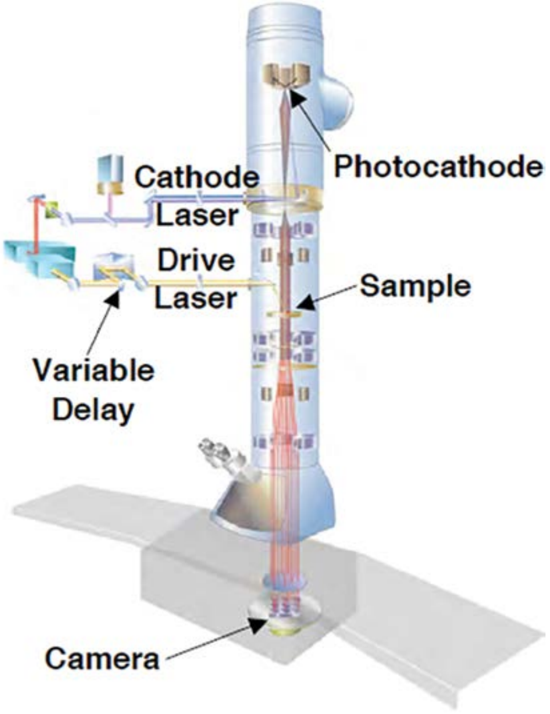

Figure 20: *A Dynamic Transmission Electron Microscope (DTEM).*

Equipment at the California Institute of Technology

Infrared Radiation Detector (High Speed Thermal Camera) – This single-point infra-red radiation detector is used to study the thermal softening that occurs by rapid heating of compressively deformed materials. Alone, the detector measures the emitted radiation of the sample. Used in conjunction with the Kolsky bar, the detector provides details of the thermal state. In-depth studies of the conversion of plastic work to heat deliver data that can be fed into continuum models.

Hooke & Zwicky Computing Clusters – Continuum simulations of Mg and Mg alloys are performed on this high-performance computing cluster. Hooke is a shared 61-node (732 total processor cores) cluster that uses code that is parallel at thread and MPI level to exploit massive parallelism of calculations. Computationally-expensive simulations can be run on Zwicky, a shared 208-node (2580 total processor cores) cluster.

Garuda Cluster – The Garuda Cluster is a high-performance computing cluster that is used for large-scale multiscale simulations of Magnesium. The cluster includes 96 dual quad core (768 total) processors with a clock speed of 2.33 GHz, 8GB RAM and 148 GB storage per node.

Equipment at Rutgers University

Spark Plasma Sintering (SPS) System – The Center for Ceramic Research building houses a 20-ton high-temperature spark plasma sintering system with mass spectrometry capabilities. The SPS system is a pressure-assisted process utilizing up to 300 tons of force. The atmosphere is vacuum with the ability to use inert gas and heat feedback is provided via thermocouples or pyrometer. The system includes programmable pressure, power settings and data acquisition.

Hot Press – The hot press' induction heating system has the ability to reach 2200°C with a maximum pressure of 20 thousand pounds per square inch. The treatment cycles are programmable to specified heating and cooling rates. The available dies can hold samples that are up to 4 inches in diameter.

Powder Synthesis System – The powder synthesis system is based on a Thermal Technologies 4560 graphite furnace with a temperature rating of 2500°C. A custom-made water-cooled copper lance allows for the rapid injection of reactants into the hot zone of the furnace, thus avoiding the reaction control issues associated with slow heating. Gas flow and thermal management is achieved through custom designed graphite components. Reactant input is controlled through a screwfeed.

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1. Garuda Cluster

Equipment at the University of Delaware

Atomic Force Microscope (AFM) – The AFM is a non-destructive imaging technique with the ability to image surfaces with nanometer resolution. The system has proven excellent for imaging a wide range of materials including composites, high performance fibers, ceramics and metals.

Wide Angle X-Ray Diffraction (WAXD) – The Wide Angle X-ray Diffraction system is equipped with a 2D detector and a copper radiation source. The WAXD is used to analyze the crystal structure of UHMWPE fibers. The 2D detector allows determination of crystal alignment relative to the fiber axis and the WAXD system itself is used to determine scattering domain size through analysis of peak breadths for respective crystal planes.

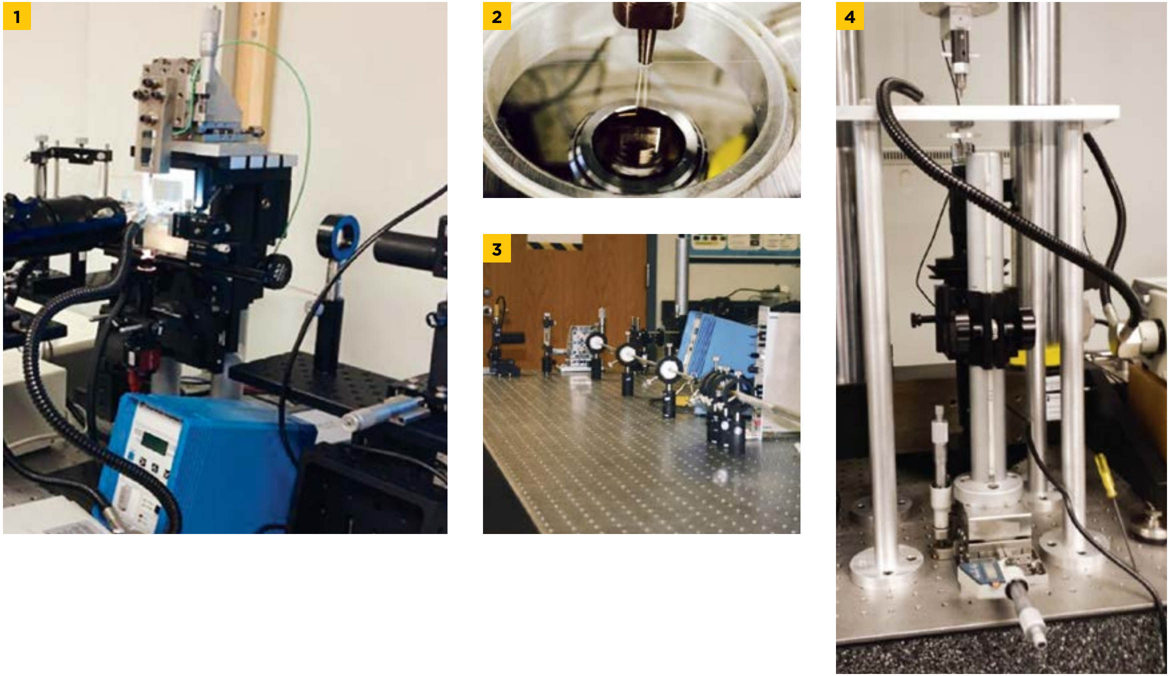
Quasi-Static and Dynamic Microdroplet Test System – The quasi-static microdroplet test setup, developed and fabricated by UD-CCM, is capable of testing at loading rates of 0.1 μm/s to 10 mm/s. To measure applied load for lower loading rates, a static load cell is used, which can be replaced by a fast response piezoelectric load cell for intermediate loading rates. In the dynamic microdroplet test setup, high rate microdroplet experiments can be performed which is based on a modified tensile Kolsky bar. This test system has been used in determining the high-strain-rate behavior of fiber-matrix interphase.

Quasi-Static Single Fiber Transverse Compression Test Setup – The quasi-static single fiber transverse compression test setup allows transverse compression of a single high performance polymer fiber with the ability to measure applied load, displacement and the compressed width of the fiber. Sapphire substrates are used as platens to compress the fibers. A 14-megapixel microscope digital camera with a pixel size of 1.4 μm×1.4 μm is used to record the deformation of single fibers.

Equipment at Washington State University

Impact Laboratory – The Institute for Shock Physics at Washington State University has three single stage, light gas guns capable of achieving projectile velocities to 1.5 km/s. One of these gas guns was built for performing combined compression and shear loading experiments. Three powder guns capable of achieving impact velocities to 2.5 km/s are also used routinely. One of these powder guns is used exclusively for x-ray diffraction measurements. To achieve higher stresses (1-2 Mbar), a two-stage, light gas gun is used to achieve impact velocities to 5 km/s.

Interferometry Systems – Time-resolved continuum measurements on shocked solids are routinely carried out using laser interferometry (VISAR – single and multi-point) systems. Interferometer components include high power narrow linewidth CW lasers, high bandwidth digitizers, high speed optical detectors and amplifiers, laser modulators, delay generators, piezo drivers/positioners, precision optics, optics tables, and laser enclosures. These measurements provide insight into the elastic-inelastic response of solids at high stresses and at very high loading rates.



1 - 4. Quasi-Static and Dynamic Microdroplet Test Setup

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ABBREVIATIONS AND ACRONYMS

ARL	Army Research Laboratory
CALTECH	California Institute of Technology
CCM	Center for Composite Materials
CCOMC	Ceramic, Composite and Optical Materials Center
CMC	Consortium Management Committee
CMEDE	Center for Materials in Extreme Dynamic Environments
CMRG	Collaborative Materials Research Group
CTRG	Collaborative Technical Research Group
DELAWARE	University of Delaware
DREXEL	Drexel University
DSTL	Defence Science and Technology Laboratory
DTEM	Dynamic Transmission Electron Microscope
EMRM	Enterprise for Multiscale Research of Materials
HEMI	Hopkins Extreme Materials Institute
JHU	Johns Hopkins University
LLNL	Lawrence Livermore National Laboratory
MEDE	Materials in Extreme Dynamic Environments
MEDE CRA	MEDE Collaborative Research Alliance
MGI	Materials Genome Intitative
MORGAN STATE	Morgan State University
NMT	New Mexico Institute of Mining and Technology
PURDUE	Purdue University
RUTGERS	Rutgers University
SEM	Scanning Electron Microscope
SWRI	Southwest Research Institute
TEM	Transmission Electron Microscope
UCSB	University of California, Santa Barbara
UHMWPE	Ultra High Molecular Weight Polyethylene
UTSA	The University of Texas at San Antonio
WSU	Washington State University

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