Mechanics of Materials and Structures (MoMS)
Design of Engineering Material Systems (DEMS)

at NSF

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National Academies, USNCTAM
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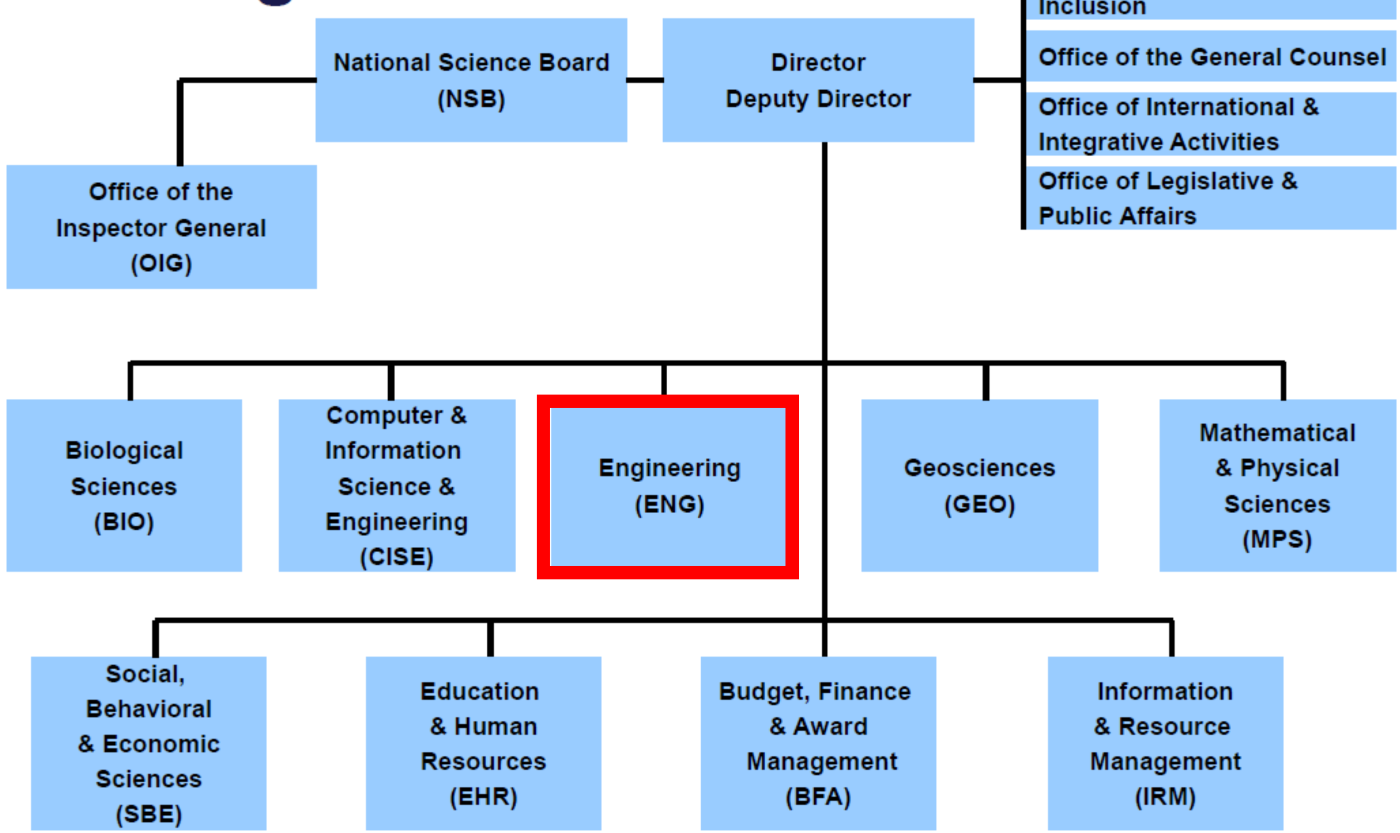
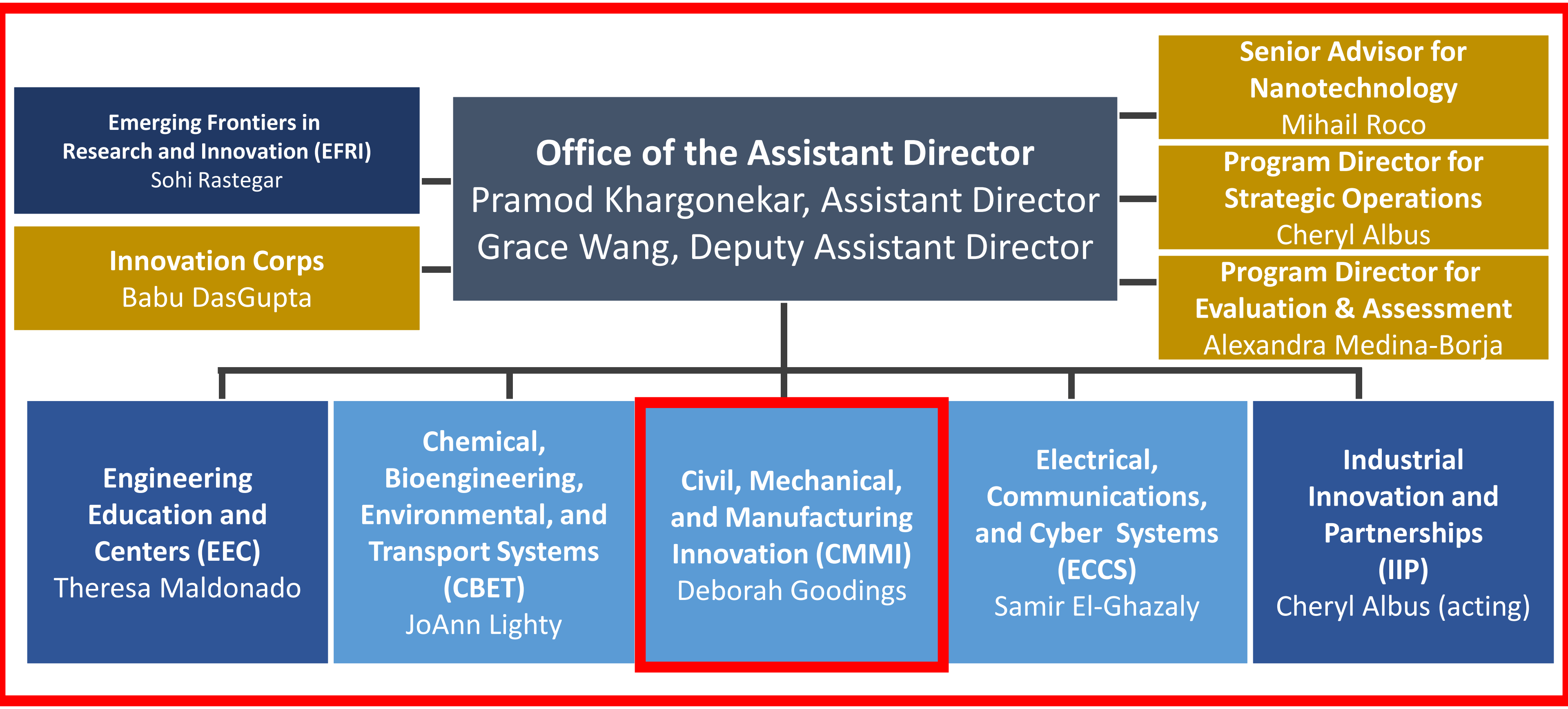
NSF Organizational Chart



NSF Directorate for Engineering (ENG)



MOMS-Synopsis

MOMS program supports fundamental research in **mechanics**

- annual budget around $12M
- emphasis on research that leads to advances in
    1) theory, experimental, and/or computational methods in mechanics,
    2) and/or uses contemporary mechanics methods to address modern challenges in materials and structures
- emphasis is primarily on making fundamental new advances at the forefront of the field of mechanics

MOMS-Synopsis

- advances in fundamental understanding of deformation, fracture, fatigue, contact and friction
- constitutive modeling, multi-scale (spatial or temporal) and multi-physics analysis, computational methods, or experimental techniques
- also structural response, not limited to
  - advances in the understanding of nonlinear deformation, instability and collapse in the context of large deformation, wave propagation
  - multi-scale (spatial or temporal) and multi-physics analysis, computational methods, or experimental techniques.

MOMS Synopsis: Opportunities

- Proposals at the intersection or considerate of the integration of material and structure are especially welcome:
    - metamaterials, hierarchical, microarchitectured and low-dimensional materials
    - address the integration and combination of geometry, topology of material distributions, length scales and deformation/failure mechanics.
- Within this context, the challenge of the notion of what constitutes a “material” or a “structure” is expected to lead to unique opportunities in terms of analysis and experimentation of novel response characteristics.

Microstructural Foundations of Magnesium Performance: A Data Mining approach to High-throughput HREBSD

David Fullwood, Mike Miles, Brigham Young University

High Resolution EBSD

Three foundational papers have recently been published that validate the simulated pattern approach to HREBSD for the first time[1], and present new methodologies for characterizing dislocations[2,3].

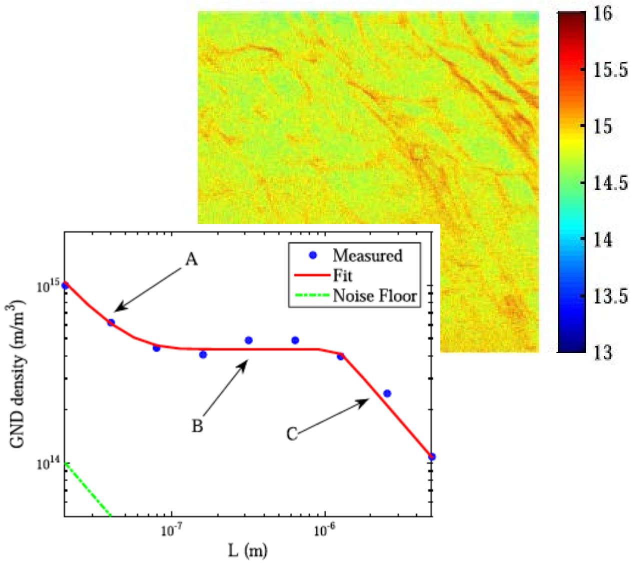


Fig. 1 GND density obtained from HREBSD (top), and identification of three distinct length-scale domains (bottom)

Data Mining EBSD

Key observations have been published relating microstructure to twin activity in Mg. Specifically, new relations between twin formation / propagation and grain boundary type have been established[4].

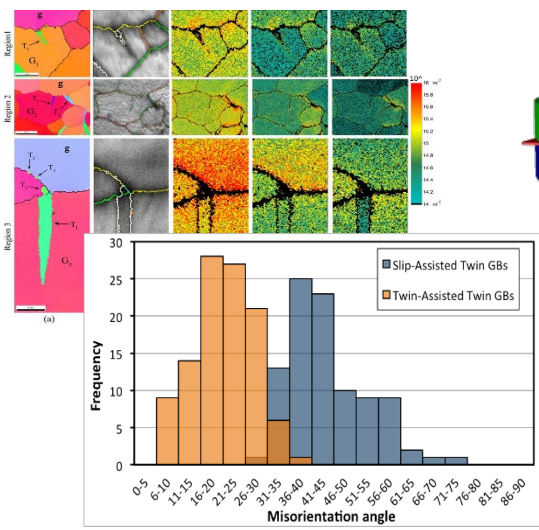


Fig. 2 IPF, IQ and GND maps in Mg, and resulting relations between twinning and GB type

Forming of Mg

Key forming tests of Mg at various temperatures have been carried out in conjunction with GM. Simulation of the test has been successfully performed, and full analysis of the data is underway.

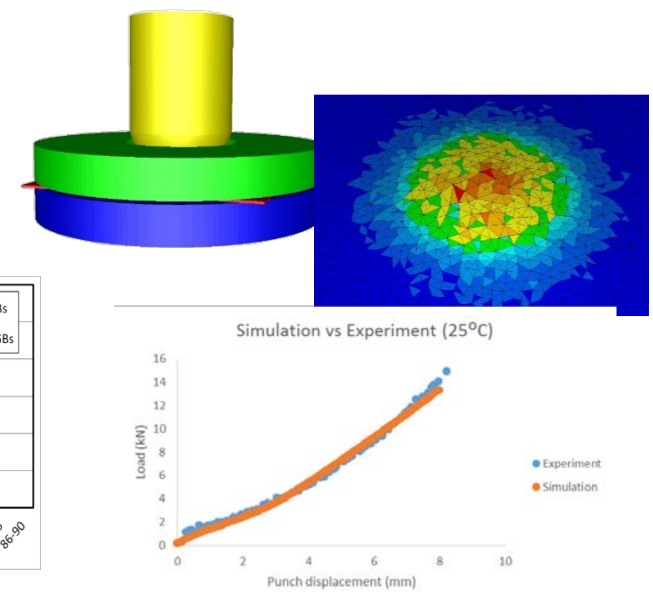


Fig. 3 FEA of LDH test, with strains matching DIC results (right) and test loads (bottom)

1. David Fullwood, Mark Vaudin, Craig Daniels, Timothy Ruggles, and Stuart I. Wright, Materials Characterization, 107 (2015), 270-277
2. T.J. Ruggles, T.M. Rampton, A. Khosravani, D.T. Fullwood, Ultramicroscopy, 164 (2016), 1-10
3. T.J. Ruggles, D.T. Fullwood, J. Kysar, International Journal of Plasticity, 76 (2016), 231-243
4. Ali Khosravani, David Fullwood, John Scott, Michael Miles, Raj Mishra, Acta Materialia, 100 (2015), 202-214

Role of symmetry in the properties of nanostructures: A first principles approach

Phanish Suryanarayana

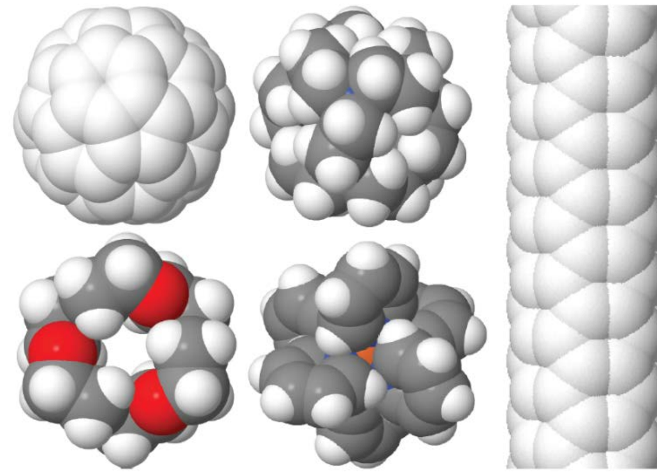
Symmetry-adapted real-space DFT

Symmetry-adapted linear-scaling DFT

Symmetry-adapted ab-initio dynamics

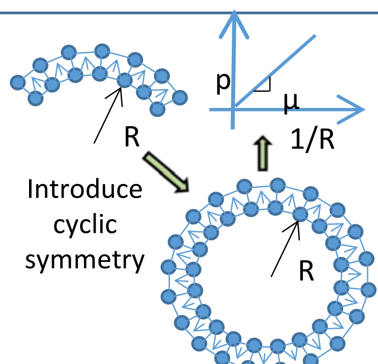
Symmetry-adapted coarse-grained DFT

Massively parallel implementation

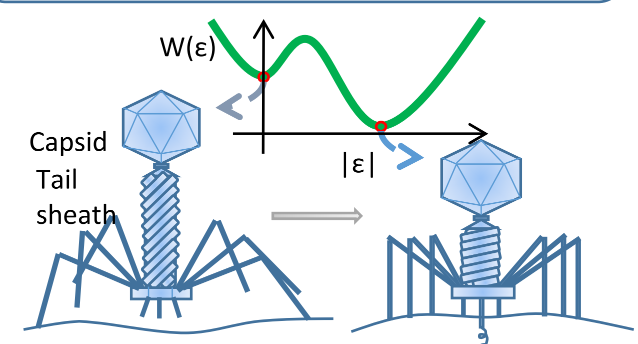


Novel symmetry-adapted ab-initio framework for Objective Structures based on Density Functional Theory (DFT)

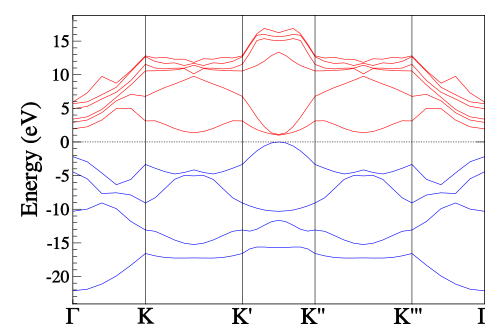
Nanoscale flexoelectricity



Phase transformation of the bacteriophage T4 tail sheath

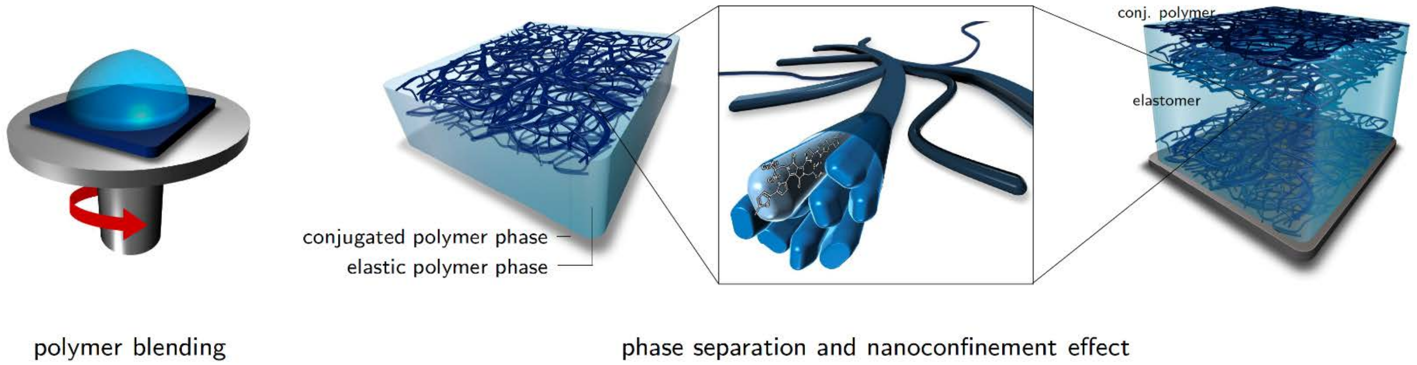


Search for linear dispersion nanostructures

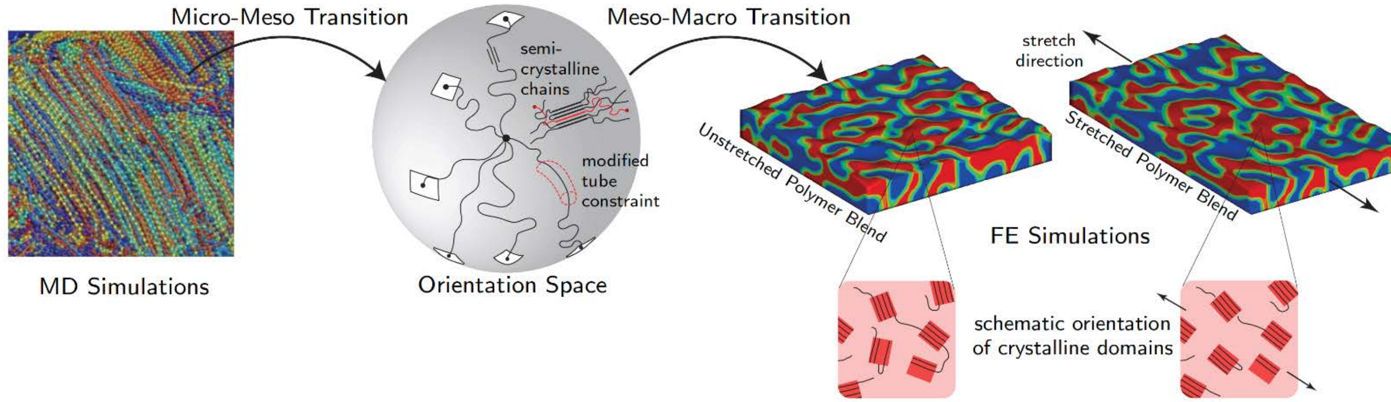


CAREER: Stretchability by Design – Understanding Mechanical Phenomena in Microarchitectured Soft Material Systems (PI: Christian Linder, Stanford University)

Illustration of Polymer Blending and Phase Separation Induced Nanoconfinement Effect



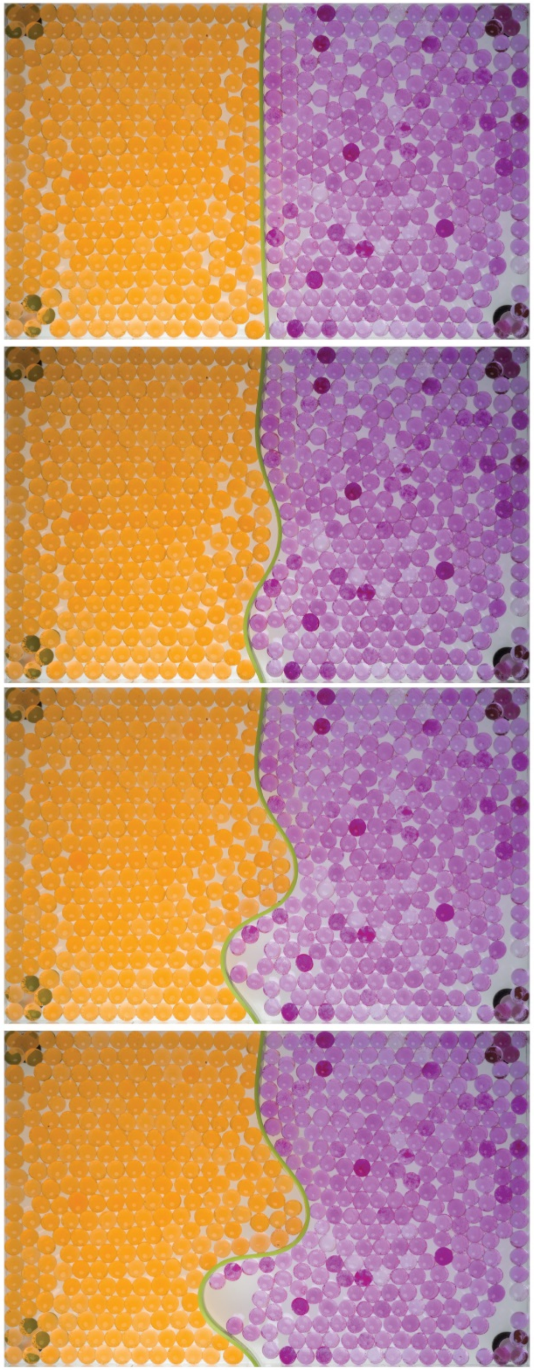
Computational Approach



Research Objectives

- Understand the mechanics of instability-driven phase separation to induce nanoconfined morphologies in conjugated/amorphous polymer blends.
- Investigate nanoconfinement mechanisms to alter mechanical properties and to tune crystalline domain alignment in polymer blends.
- Propose new failure mechanisms to describe the onset and propagation of failure zones within the microarchitectured soft material system.

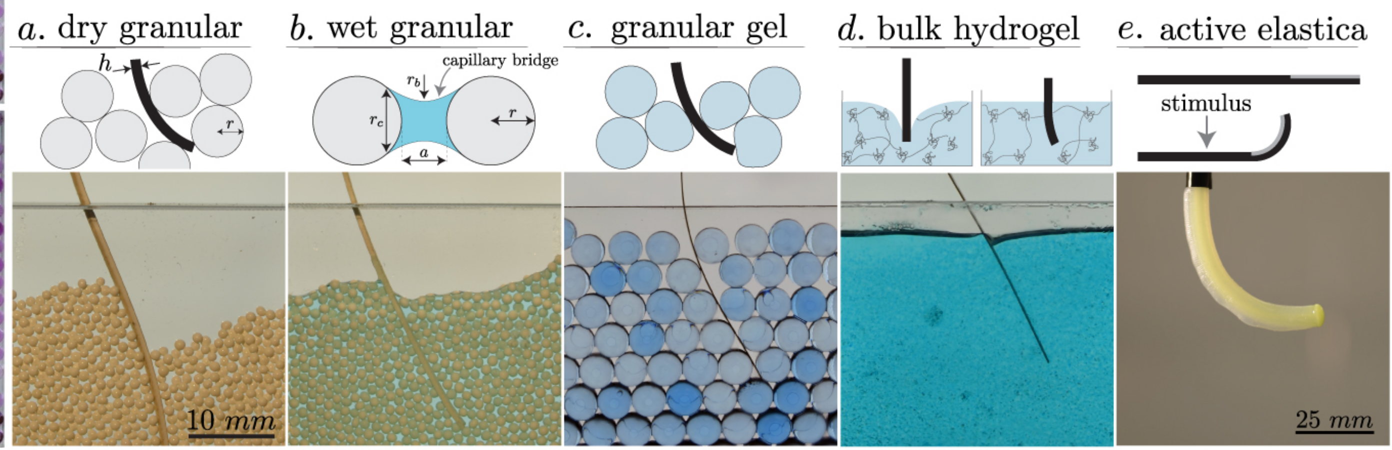
CAREER CMMI-1454153: Understanding and Controlling the Deformation of Thin Rods within Soft and Fragile Matter



Douglas P. Holmes, Boston University

Intellectual Merit

What governs the **mechanics** of a burrowing, flexible structure, and can the incorporation of advanced materials lead to ‘smart’ structures capable of navigating complex media with precision?



Broader Impacts

Can we improve scientific communication and literacy by utilizing online digital media to inspire, educate, and communicate science to the broader global community?

Products

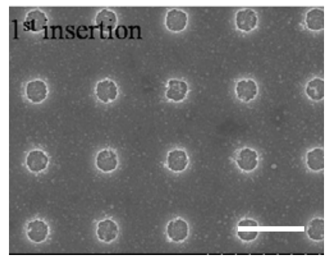
1. A.R. Mojdehi, B. Tavakol, W. Royston, D.A. Dillard, and D.P. Holmes, “Buckling of elastic beams embedded in granular media,” *Extreme Mechanics Letters*, doi:10.1016/j.eml.2016.03.022, (2016).
2. D.P. Holmes, Mechanics of Materials: Online, www.bu.edu/moss/courses, (2016).

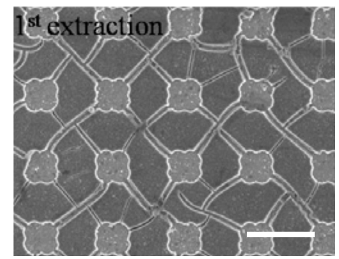
CAREER: In Situ Nanomechanics of High-Performance Anode Materials for Sodium-Ion Batteries (Georgia Tech: Shuman Xia)

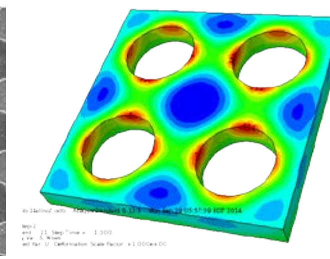
Goal:

- Develop a novel experimental platform for characterizing the **mechanical** response of NIB electrode materials during **electrochemical** reaction

Integrated experiments and predictive modeling of phase and morphological evolution in high-performance NIB electrodes

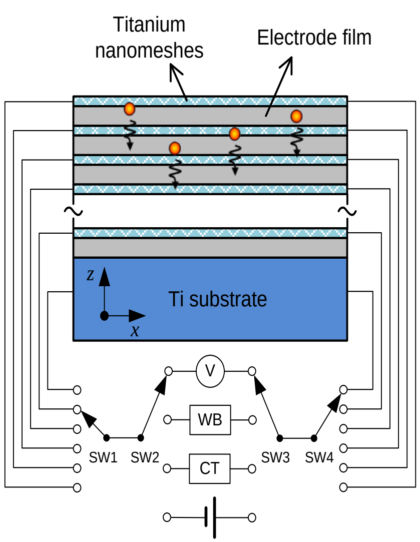




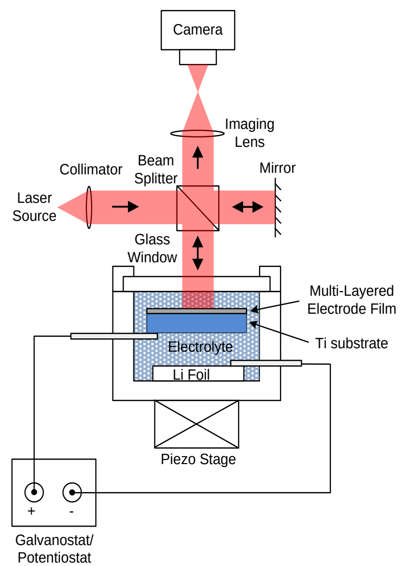


A novel nanomechanical test platform for electrode material characterization

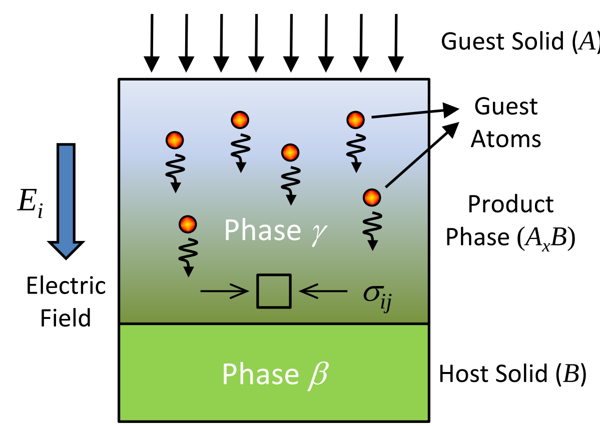
(a)



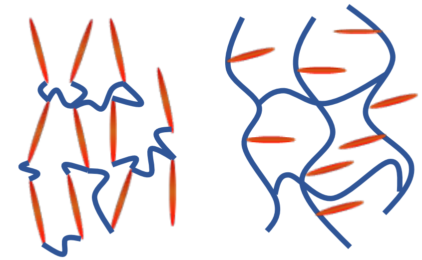
(b)



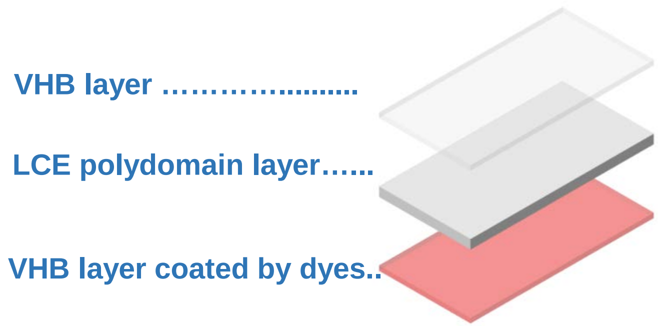
Characterizations of Na diffusion & reaction, coupled with large deformation and high stress

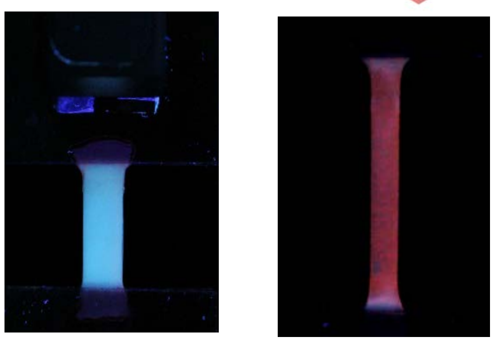


CAREER: Experimental and Theoretical Studies of Mechanics Interacting with Electric/Optical Fields in Liquid Crystal Elastomers



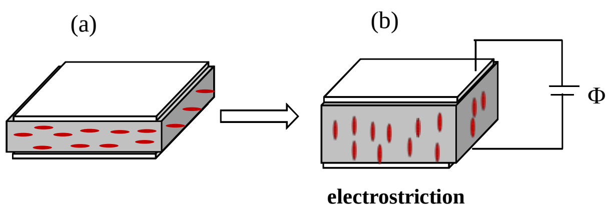
Mechanochromic LCE structures





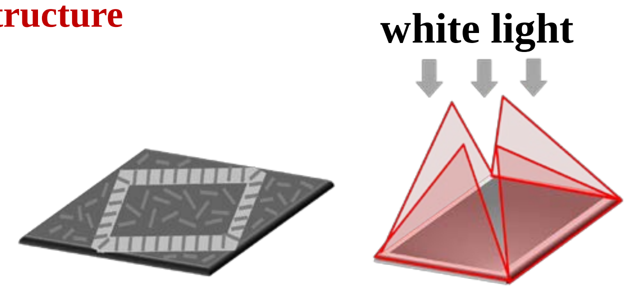
Stretch-induced color change

Novel Voltage-induced deformation in LCEs



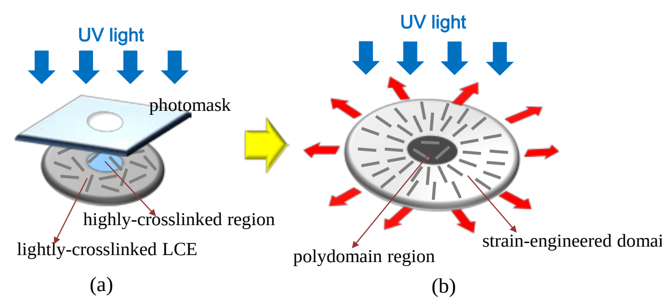
Giant electrostriction

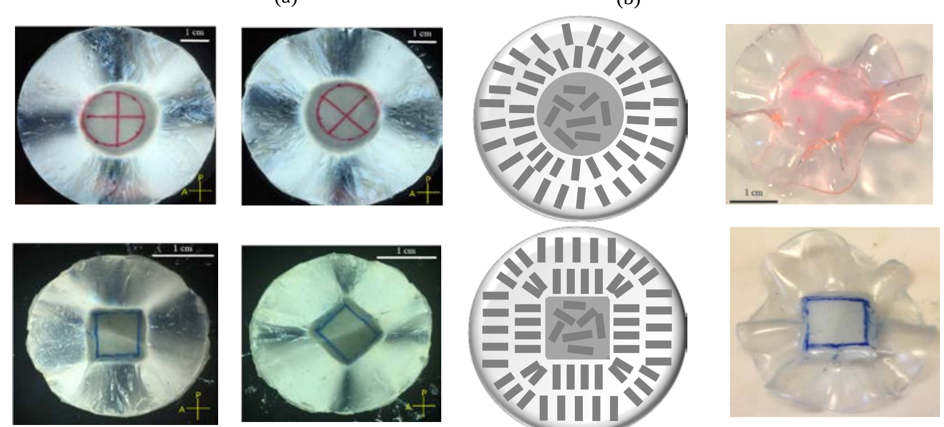
Light-induced active deformation in a LCE structure



Light-induced folding

Patterning LCE through self-developed strain engineering technique

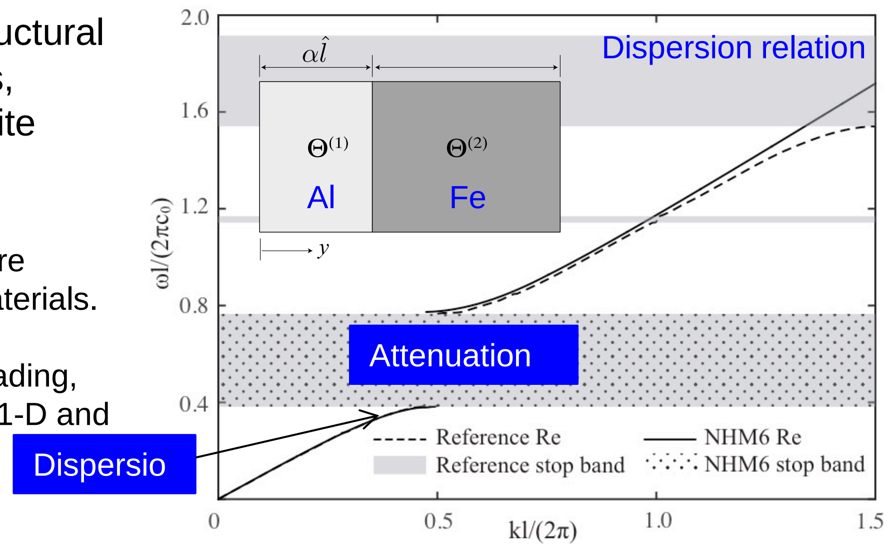




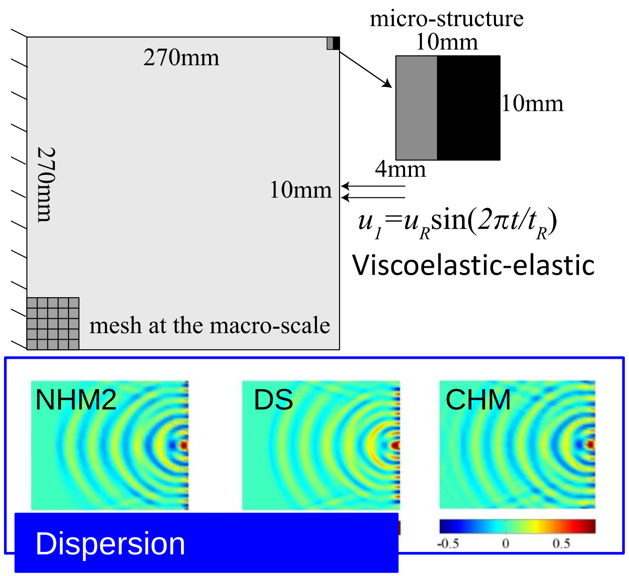
Molecular patterning through applying inhomogeneous stretch

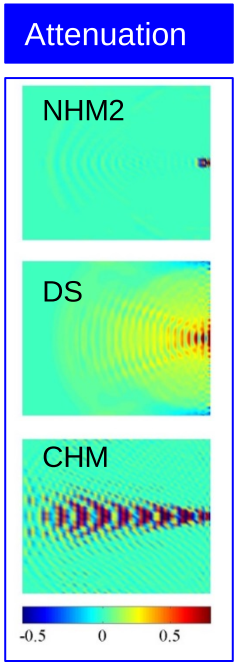
Mechanics and Dynamics of Viscoelastic Metacomposites

- **Project Goal:** Establish relationships between microstructural morphology, viscoelastic constituent material parameters, energy dissipation and wave attenuation in metacomposite materials.
- **Recent Scientific Accomplishments:**
  - Developed multiscale computational models that can capture dispersive and band structure in elastic and viscoelastic materials.
  - Developed the ability to perform time domain analysis of metacomposite structural systems subjected to dynamic loading, taking into effect the dispersive and dissipative behavior in 1-D and 2-D.
- **Broader Impacts:**
  - The proposed research allows the assessment of the true performance of structures made of metacomposites through full scale analysis.

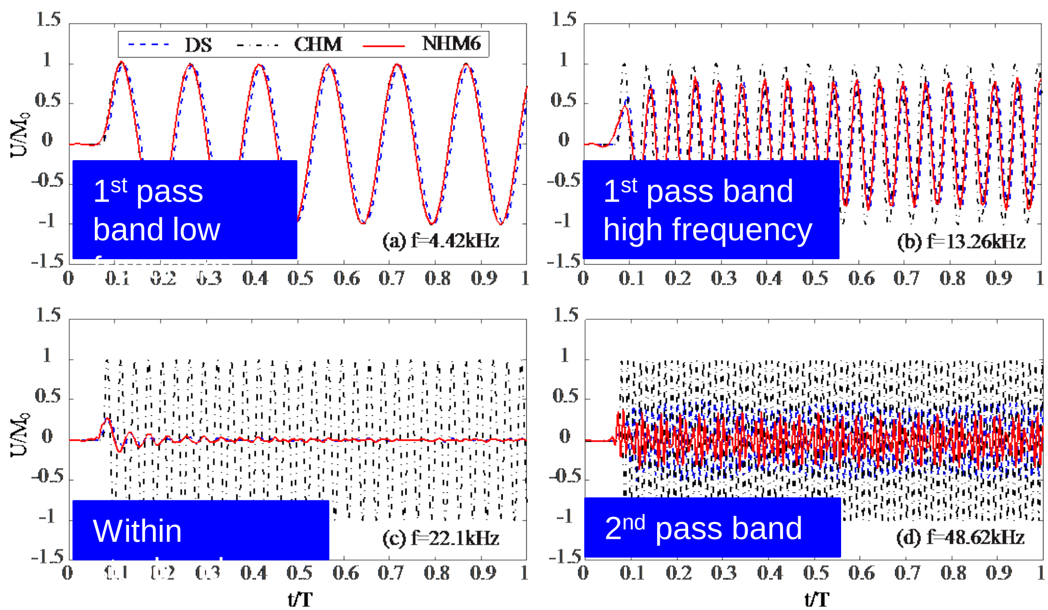


Multidimensional analysis





1D-case Time domain response

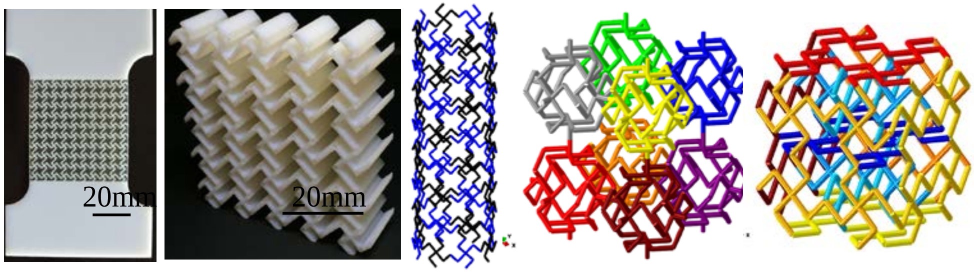


NHM: Proposed model CHM: Classical homogenization model DS: Direct simulations

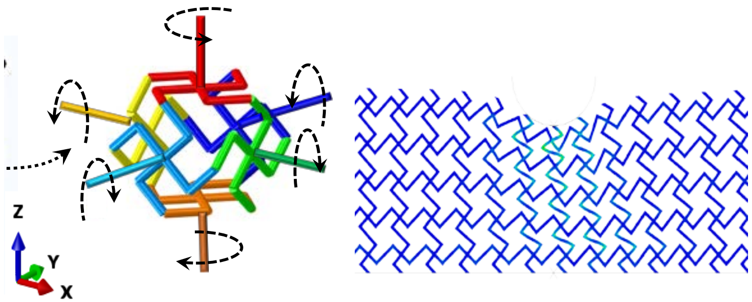
Mechanics of a New Family of Auxetic Chiral Composites (NSF/CMMI/MoMS #1554468)

PI: Yaning Li, University of New Hampshire

- **A new family of auxetic chiral composites**
  - New 2D & 3D designs
  - Auxetic effect under large deformation
  - Deformation with large internal rotation
  - New deformation mechanisms
  - Integrate mechanics and 3D printing



- **The coupled auxetic and chiral effects, probed by micropolar theory**
  - Use the new designs to advance micropolar thoery
  - Solve the first and second planar problems
  - Implementation and experimental verification



- **Education plan and broad impact**
  - New England STEM education, supporting "Next Generation Science Standards (NGSS)"
  - Collaboration with local industries
  - Broad participation, increasing diversity

Design of Engineering Material Systems (DEMS)

DEMS supports fundamental research intended to lead to new paradigms of design, engineering, and insertion of advanced engineering material systems.

Integrates theory, processing/manufacturing, data/informatics, experimental, and/or computational approaches with **rigorous engineering design principles.**

Annual budget around $3 M

Complete program description available at:
https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504809

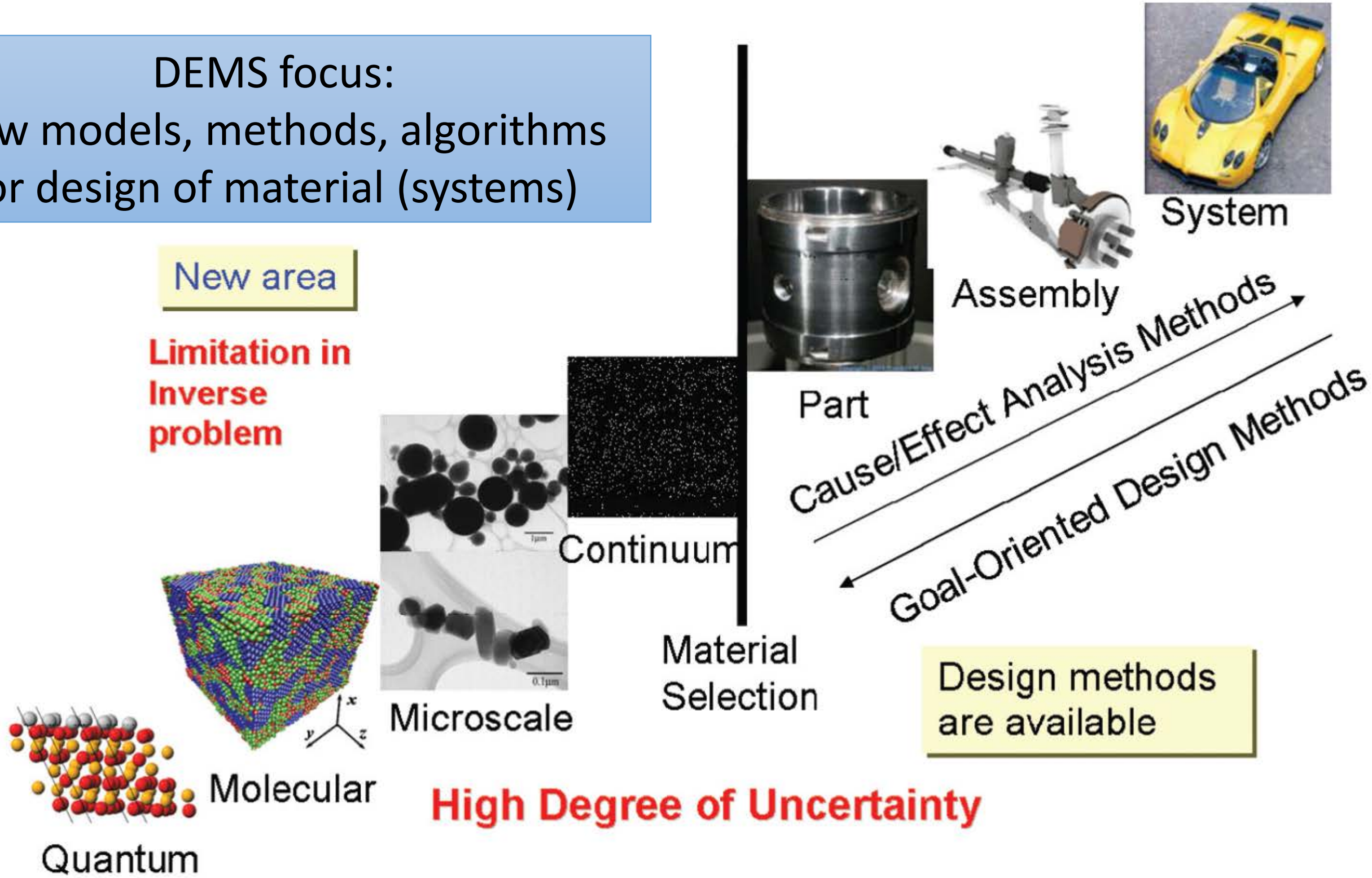
DEMS Staff

- Chris Paredis
  - Engineering Systems Design, Systems Science
- Mary Toney
  - Materials Engineering and Processing
- Kara Peters
  - Mechanics of Materials and Structures

Questions can be submitted
by email: **dems@nsf.gov**

Why DEMS?
— Intellectual Challenges

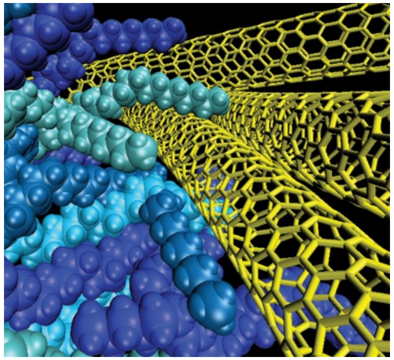
DEMS focus:
New models, methods, algorithms for design of material (systems)



McDowell, Olsen. "Concurrent design of hierarchical materials and structures," Sci Model Simul (2008) 15:207-240.

Why DEMS?
— Benefits to Society

- Materials research can now measure and observe phenomena at unprecedented length and time scales
- Society benefits when these capabilities are realized within actual engineered products
- Deliver new levels of system performance through integrated *<u>material systems</u>* development



Carbon Nanotube
Reinforced Composite
Image Courtesy
ALTEC SpA

Tesla S
Image Courtesy
MotorAuthority

Artificial Heart Valve
Image Courtesy
Wikipedia Commons

What is Design?

— Design is a Purposeful Activity

- What is the purpose of the design process?
  - To obtain a state of the world that **is more preferred**
  - To **add value**

- How do we **add value**?
  - By creating or improving artifacts — in this case: materials

- Rather than realizing the artifact, designers **specify a plan – a model –** for how to realize the artifact. Models are used to:
  - Specify a plan for how to realize the artifact/material
  - Predict the consequences of executing the plan

Find a specification for the realization of a material system with desired properties — properties that are preferred/valuable

Examples of Potentially Promising Search Strategies

- ***Models at different levels of abstraction***
  - Inexpensive but less accurate models for global exploration; more accurate but expensive models/experiments for local optimization

- ***Decomposition and parallelization***
  - Decompose the problem into multiple decisions that may be pursued both sequentially or in parallel

- ***Consider uncertainty explicitly***
  - To allow for effective pruning of search trees and planning of efficient gathering of additional information

Outcomes of a Good DEMS Proposal

- Advance the state of knowledge of materials design methodology
  - New modeling formalisms for abstracting material systems (at different levels of abstraction) specifically well-suited for design
  - New algorithms for searching materials design spaces; characterization of the efficiency of such algorithms
  - Adaptations of existing formalisms and algorithms to materials design
  - Approaches for capturing/representing (rather than just collect) materials domain knowledge so that it becomes useful for design
  - …

Discovering a new material in the course of your project could be a strong broader impact, but by itself, does not contribute to the state of knowledge of materials-design methods — it is therefore not a required outcome

Optimal Design in Multifunctional Space

Design of Negative Stiffness Metamaterials; PI Seepersad

Bayesian Network classifiers in materials design, map promising designs and for classification of solution spaces