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4. TITLE AND SUBTITLE Multi-scale hierarchical and topological design of structures for failure resistance			5a. CONTRACT NUMBER W911NF-10-1-0127		
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6. AUTHORS Markus J. Buehler			5d. PROJECT NUMBER		
			5e. TASK NUMBER		
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14. ABSTRACT The goal of this project was the computational and theoretical analysis and synthesis of failure mechanisms in hierarchical structures and materials found in biology's structural materials, and the transfer of the results towards the design of hierarchical bioinspired heteronano-composites. By developing and applying a model that couples atomistic to mesoscopic scales, the major outcomes of this basic research project are: (i) the systematic analysis of deformation and failure mechanisms in biological hierarchical structures (such as bone and spider silk), (ii) the					
15. SUBJECT TERMS Composites, materials, simulation, 3D printing, advanced manufacturing, design, fracture					
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a. REPORT UU	b. ABSTRACT UU	c. THIS PAGE UU			19b. TELEPHONE NUMBER 617-452-2750

Report Title

Multi-scale hierarchical and topological design of structures for failure resistance

ABSTRACT

The goal of this project was the computational and theoretical analysis and synthesis of failure mechanisms in hierarchical structures and materials found in biology's structural materials, and the transfer of the results towards the design of hierarchical bioinspired heteronanocomposites. By developing and applying a model that couples atomistic to mesoscopic scales, the major outcomes of this basic research project are: (i) the systematic analysis of deformation and failure mechanisms in biological hierarchical structures (such as bone and spider silk), (ii) the development of designs for heterogeneous materials involving variations in hierarchical structure and topology for damage tolerance, (iii) the development of multiscale models describing the mechanics of materials with disordered heterogeneous distributions of mechanical properties with the potential of uncertainty quantification of fracture properties, and (iv) the development of a hierarchical model that captures deformation mechanisms at multiple hierarchical levels, resulting in hierarchical Ashby deformation mechanism design maps. The project also aims at developing methods to realize physical samples for testing, which reflect the designed geometries.

This project addressed a critical frontier in engineering science, the optimization of nanostructure, mesostructure and topological features for failure properties. Whereas structural optimization at larger length-scales has been employed earlier, a systematic investigation of the adaptation of hierarchical nanostructures for failure properties under extreme mechanical loading has not been reported. Moreover, a novel approach offers the possibility of characterizing uncertainties in material properties with the view towards a rigorous risk assessment of the fracture response of advanced hierarchical composites. This work is crucial for the U.S. Army as it may lead to a new engineering paradigm to enable the design of novel protective coatings, helmets or textiles. Resulting models will be made available to ARL and other DOD researchers. Overall, the progress has been great and opened very new directions for future research, which has been received extremely well by our peers and the academic community. Novel elements related to uncertainty quantification have been developed recently, which could bring high-impact applications to the work.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

<u>Received</u>	<u>Paper</u>
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08/29/2012	9.00 Leon S Dimas, Markus J Buehler. Influence of geometry on mechanical properties of bio-inspired silica-based hierarchical materials, Bioinspiration & Biomimetics, (09 2012): 36024. doi: 10.1088/1748-3182/7/3/036024
08/29/2012	11.00 Steven W. Cranford, Anna Tarakanova, Nicola M. Pugno, Markus J. Buehler. Nonlinear material behaviour of spider silk yields robust webs, Nature, (02 2012): 0. doi: 10.1038/nature10739
08/29/2012	10.00 Max Solar, Markus Buehler. Taking a leaf from nature's book, Nature Nanotechnology, (07 2012): 417. doi:
08/30/2011	1.00 Dipanjan Sen, Markus J. Buehler. Structural hierarchies define toughness and defect-tolerance despite simple and mechanically inferior brittle building blocks, Scientific Reports, (7 2011): 35. doi: 10.1038/srep00035
08/30/2011	4.00 D. Sen, M. Buehler. ATOMISTICALLY-INFORMED MESOSCALE MODEL OF DEFORMATION AND FAILURE OF BIOINSPIRED HIERARCHICAL SILICA NANOCOMPOSITES, International Journal of Applied Mechanics, (06 2010): 699. doi:
08/30/2011	3.00 Andre Garcia, Nicola Pugno, Markus J Buehler. Superductile, Wavy Silica Nanostructures Inspired by Diatom Algae, Advanced Biomaterials, (11 2011): 0. doi:
08/30/2011	2.00 Tuomas Knowles, Markus Buehler. Nanomechanics of functional and pathological amyloid materials, Nature Nanotechnology, (08 2011): 460. doi:
08/31/2011	5.00 A.P. Garcia, D. Sen, M.J. Buehler. Hierarchical silica nanostructures inspired by diatom algae yield superior deformability, toughness and strength, Metallurgical and Materials Transactions, (1 2011): 0. doi:
08/31/2011	8.00 D. Sen, A. Garcia, M.J. Buehler. Mechanics of nano-honeycomb silica structures: A size-dependent brittle-to-ductile transition, Journal of Nanomechanics and Micromechanics (ASCE), (11 2011): 0. doi:
08/31/2011	6.00 I. Mohedas, A. Garcia, M.J. Buehler. Nanomechanics of biologically inspired coiled silica nanostructures, Proceedings of the Institution of Mechanical Engineers, Part N: Journal of Nanoengineering and Nanosystems, (07 2011): 0. doi:
10/04/2013	13.00 Leon S. Dimas, Markus J. Buehler. Tough and stiff composites with simple building blocks, Journal of Materials Research, (05 2013): 0. doi: 10.1557/jmr.2013.88
10/04/2013	14.00 Leon S. Dimas, Graham H. Bratzel, Ido Eylon, Markus J. Buehler. Tough Composites Inspired by Mineralized Natural Materials: Computation, 3D printing, and Testing, Advanced Functional Materials, (09 2013): 0. doi: 10.1002/adfm.201300215
10/04/2013	15.00 Leon Dimas, Tristan Giesa, Markus J. Buehler. Fracture in stochastic media using discrete and continuum simulation methods, Journal of the Mechanics and Physics of Solids, (10 2013): 0. doi:
10/04/2013	16.00 Alfonso Gautieri, Shu-Wei Chang, Arun K. Nair, Markus J. Buehler. Molecular mechanics of mineralized collagen fibrils in bone, Nature Communications, (04 2013): 0. doi: 10.1038/ncomms2720

TOTAL:	14
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Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Paper

08/29/2012 12.00 Steve Cranford, Markus Buehler. Biomateriomics, New York: Springer, (06 2012)

08/31/2011 7.00 D. Sen, M.J. Buehler, A. Garcia. Nature's flexible and tough armor: Geometric and size effects of diatom inspired, nanoscale glass, Baco Raton, FL: CRC PRes, (01 2012)

TOTAL: 2

Patents Submitted

Patents Awarded

Awards

-TMS Hardy Award 2013

-2012 TMS Structural Materials Division JOM Best Paper Award

-Chair, Fifth International Conference on Mechanics of Biomaterials & Tissues 2013, Sitges, Spain (December 2013)

-Co-Chair, NanoEngineering in Medicine and Biology Congress (NEMB 2013), Boston, 2013 (February 2013)

-PI was promoted to Full Professor, effective July 1, 2013

-PI was named Head of the Department of Civil and Environmental Engineering, July 1, 2013

Graduate Students

<u>NAME</u>	<u>PERCENT_SUPPORTED</u>	<u>Discipline</u>
Leon Dimas	0.80	
Tristan Giesa	0.20	
David Adler	0.00	
Dipanjan Sen	1.00	
FTE Equivalent:	2.00	
Total Number:	4	

Names of Post Doctorates

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Zhao Qin	0.25
FTE Equivalent:	0.25
Total Number:	1

Names of Faculty Supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Markus J. Buehler	0.05	
FTE Equivalent:	0.05	
Total Number:	1	

Names of Under Graduate students supported

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:.....	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):.....	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:.....	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Dipanjan Sen

Total Number: 1

Names of other research staff

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
-------------	--------------------------

FTE Equivalent:

Total Number:

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

The key novel element of this project is the use of atomistic based multi-scale modeling to explore the opportunities and potential of including the atomistic, molecular and mesoscale structure in the engineering design space by an integrated treatment of structure and material (see, e.g. M.J. Buehler and T. Ackbarow, *Materials Today*, 2007; Ackbarow et al., *PNAS*, 2007; M.J. Buehler and Y.C. Yung, *Nature Materials*, 2009; M. Buehler, *Nano Today*, 2010; Buehler et al., *Biomateriomics*, 2012).

This analysis is facilitated by using a systematic application of atomistic based multi-scale simulation to investigate how atomistic structures influence a material's performance under rapid deformation, and specifically, how hierarchical structures can be used to tune the mechanical (and in particular failure) properties of the material. This approach provides a fundamental description of the material behavior from an atomistic perspective. Our project is based on the idea of studying the sensitivities of multi-scale structural features on the material's mesoscale/macroscale performance, across the scales. The focus on multi-scale effects in the deformation mechanics of materials is an innovative idea that may lead to a new materials engineering paradigm that unifies structural and materials engineering.

The study of biological materials and structures provides us with insight into how to link the nanoscale to the macroscale. This novel viewpoint, integrating the study of biological materials with engineered materials, provides an innovative path to develop a new class of strong, robust (tough), adaptable, self-healing and multifunctional materials.

The work is of relevance to the Army for several reasons. First, the proposed research is critical on the path to develop a new engineering paradigm, with lasting effects for future materials and structure design concepts. Second, the proposed work is at the forefront of engineering science, and the investment of ARO into this type of work is crucial to sustain America's technological and scientific leadership. By involvement in this research project, ARL engineers and scientists will have access to the scientific foundation for transformational science, which could play key role in the design of future Army systems. Since tomorrow's soldier will have much greater complexity of materials, new structures must be engineered throughout multiple length-scales. In this context, the knowledge of the paradigm, scientific approach and integration into training of current and potential ARL scientists is of utmost importance to ensure a transition from cutting edge university research towards Defense applications. Mechanisms to address these issues are lectures at ARL and participation in ARL/ARO workshop. The PI is committed to contribute to this effort and considers this as a central and important theme of his research program.

SUMMARY OF PROGRESS

This project started in June 2010, and since then we have made substantial progress. Recent work focuses on the analysis of topological effects of composite design, 3D printing of bioinspired and computationally designed samples, imaging, and additional theoretical analyses. The link between topology and performance coupled with simple but insightful model systems is a hallmark of this project.

Below we summarize progress in key areas of the project.

Tough and Strong Composites with Simple Building Blocks

From bone to dentin to nacre, biomaterials are structurally advanced composites with superior toughness and superior strength, based on simple building blocks. Here, using a series of molecular mechanics models with bioinspired topologies, we propose design mechanisms rooted in the simplest mechanical interactions – perfectly brittle linear elastic – which are shown to be sufficient to achieve superior toughness and strength in biological composites. In a two-phase composite system, we show that by adapting the elastic constitutive laws of the matrix phase and by tuning the interactions of the constituents we can realize materials with a large range of combinations of toughness and strength. Notably, this can be achieved without changing the fracture energy of the individual composite components. Through a systematic analysis and the development of a simple model, we unveil fundamental design principles that lead to fundamental insight into the mechanics of natural composites for applications in a range of engineering disciplines.

A manuscript has recently been submitted and is currently under consideration at *J. Mat. Res.*:

L. Dimas, M.J. Buehler, "Tough and Strong Composites with Simple Building Blocks," *J. Mat. Res.*, in revision

Influence of geometry on mechanical properties of bio-inspired silica-based hierarchical materials

Diatoms, bone, nacre and deep-sea sponges are mineralized natural structures found abundantly in nature. They exhibit mechanical properties on par with advanced engineering materials, yet their fundamental building blocks are brittle and weak. An intriguing characteristic of these structures is their heterogeneous distribution of mechanical properties. Specifically, diatoms exhibit nanoscale porosity in specific geometrical configurations to create regions with distinct stress strain responses, notably based on a single and simple building block, silica. The study reported here, using models derived from first principles based

full atomistic studies with the ReaxFF reactive force field, focuses on the mechanics and deformation mechanisms of silica based nanocomposites inspired by mineralized structures. We examine single edged notched tensile specimens and analyze stress and strain fields under varied sample size in order to gain fundamental insights into the deformation mechanisms of structures with distinct ordered arrangements of soft and stiff phases. We find that hierarchical arrangements of silica nanostructures markedly change the stress and strain transfer in the samples. The combined action of strain transfer in the deformable phase, and stress transfer in the strong phase, acts synergistically to reduce the intensity of stress concentrations around a crack tip, and renders the resulting composites less sensitive to the presence of flaws and leads to stable crack propagation, if it occurs. A systematic study allows us to identify composite structures with superior fracture mechanical properties relative to their constituents, akin to many natural biomineralized materials that turn the weaknesses of building blocks into a strength of the overall system.

A paper has just appeared in a peer-reviewed journal:

L. Dimas, M.J. Buehler, "Influence of geometry on mechanical properties of bio-inspired silica-based hierarchical materials," *Bioinspiration & Biomimetics*, Vol. 7, paper # 036024, 2012

Fracture in stochastic media using discrete and continuum simulation methods

Experimental and computational work suggests that the heterogeneous distribution of mechanical properties in natural and synthetic materials induces a toughening mechanism that leads to a more robust structural response in the presence of cracks, defects or other types of flaws. Motivated by these results, we model an elastic solid with a Young's modulus distribution described by a Gaussian process, representing the heterogeneity in the system. We then study the pristine system using both a continuum model and a discrete perspective to establish a link between the microscale and the macroscale in the presence of disorder. Furthermore, we analyze a flawed discrete particle system and investigate the influence of heterogeneity on the fracture mechanical properties of the solid. We vary the variability and correlation length of the Gaussian process, thereby gaining fundamental insights into the effect of heterogeneity and the essential length scales of heterogeneity critical to enhanced fracture properties. Similarly to effects documented for composites with complex hierarchical architectures we find that materials with disordered elastic fields toughen by a 'distribution-of-weakness' mechanism inducing crack arrest and stress delocalization. For the particular forms of disorder investigated here, the toughness modulus can increase by up to 30 percent due to an increase in variability in the elastic field. Our work lays the foundation for stochastic modeling in a particle based micromechanical environment and unveils mechanisms by which mechanical behavior can be tailored due to increasingly heterogeneous mechanical properties.

A manuscript has recently been submitted and is currently under consideration at JMPS.:

L. Dimas, T. Giesa, M.J. Buehler, "Fracture in stochastic media using discrete and continuum simulation methods," JMPS, in submission

Tough Composites Inspired by Mineralized Natural Materials: Computation, 3D printing and Testing

Composites play an important role as structural materials in a range of engineering fields due to their potential to combine the best mechanical properties of their constituents. In biology, composites are ubiquitous and exhibit fascinating and precise architectures at fine length scales, where bone, hexactinellid sponges and nacreous abalone shells are prime examples. Here, we emulate typical biological composite topologies with multi-material 3D printing at micrometer resolution. From base materials that are brittle and exhibit catastrophic failure, we create synthetic composites with superior fracture mechanical properties exhibiting deformation and fracture mechanisms reminiscent of mineralized biological composites. Our complementary computational model predictions of fracture mechanisms and trends in mechanical properties are in good agreement with the experimental findings. The reported findings confirm that specific topological arrangements of soft and stiff phases as a design mechanism enhances the mechanical behavior in composites. This study demonstrates 3D printing as a means to create fracture resistant composites. Moreover, our results indicate that we can use computer models to design composite materials to exhibit tailored fracture properties and then use 3D printing to synthesize materials with such mechanical performance.

L. Dimas, G. Bratzel, I. Eylon, M.J. Buehler, "Tough Composites Inspired by Mineralized Natural Materials: Computation, 3D printing and Testing," *Advanced Functional Materials*, 2013

These and other recent developments are summarized in the attached set of slides.

Technology Transfer

Prof. Markus Buehler (MIT), 36 Months, FY10-FY13, ARO Core Programs, \$282,062

Objectives

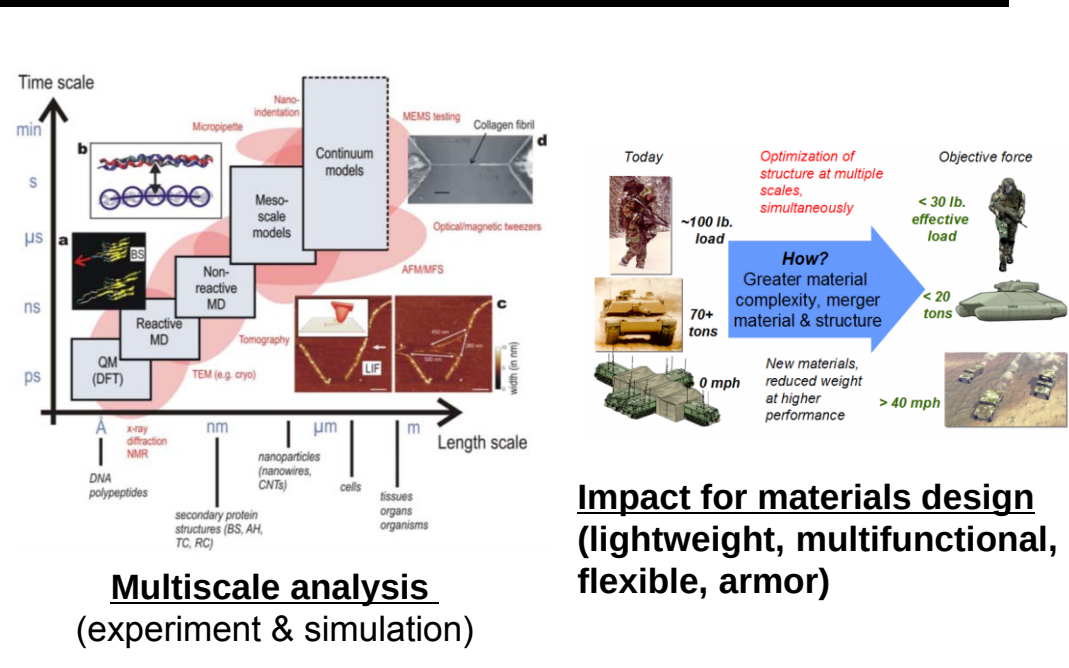
- ✓ Develop hierarchical materials that resist brittle fracture and redistributes loading energy towards dissipation in large volumes.

Scientific Challenges

- ✓ Current designs limited to single scale and no optimization for failure properties
- ✓ Identify material solutions from biology how to develop effective armor materials, from simple building blocks
- ✓ Merge structure and material, seamlessly

Accomplishments

- Elucidated influence of hierarchical topologies on the fracture response of composites
- Designed tough composites with large scale load redistribution from simple building blocks
- Developed multiscale model to analyze the mechanics of materials with disordered mechanical properties
- Synthesized tough bio-inspired composites from simple building blocks with rapid manufacturing



Army Impact

Results of this research will enable the **next-generation of composites**, and enable a new engineering paradigm to design of novel protective coatings, helmets or textiles. The work will also lead to **new lightweight ultra-tough structural materials**. Demonstrates: **MATERIALS BY DESIGN**

Funding profile: FY11-FY14 \$282,062
Email: mbuehler@MIT.EDU

Multi-scale hierarchical and topological design of structures for failure resistance

Markus Buehler, MIT, SI, \$282K, 36 Mo., 3rd year

■ Project Goal

Develop hierarchical materials using 3D printing that resist brittle fracture and redistributes loading energy towards dissipation in large volumes

■ Scientific Challenges

Identify material solutions from biology on how to develop effective armor materials, from simple building blocks

■ Uniqueness of approach

- Extend current state of the art by providing a fundamental description of material behavior under impact (cracking, plasticity, shear)
- Emulate typical biological composite topologies with multi-material 3D printing at micrometer resolution
- Combine multiscale modeling with experiment in “materials by design” (relevance for other initiatives, such as the **Materials Genome Initiative**) 2

• Objective

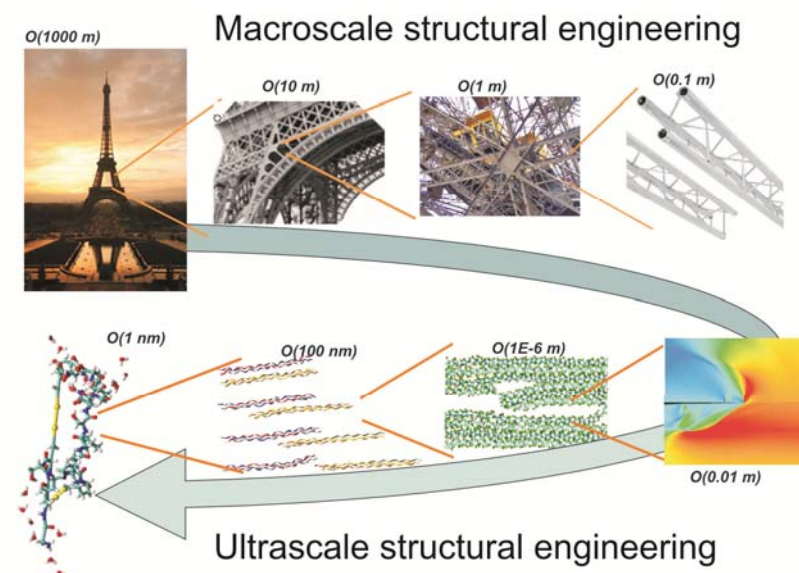
- Develop **hierarchical materials** that **resist fracture** (e.g. brittle cracking) and **redistributes loading energy** towards dissipation in large volumes

• Project Goal

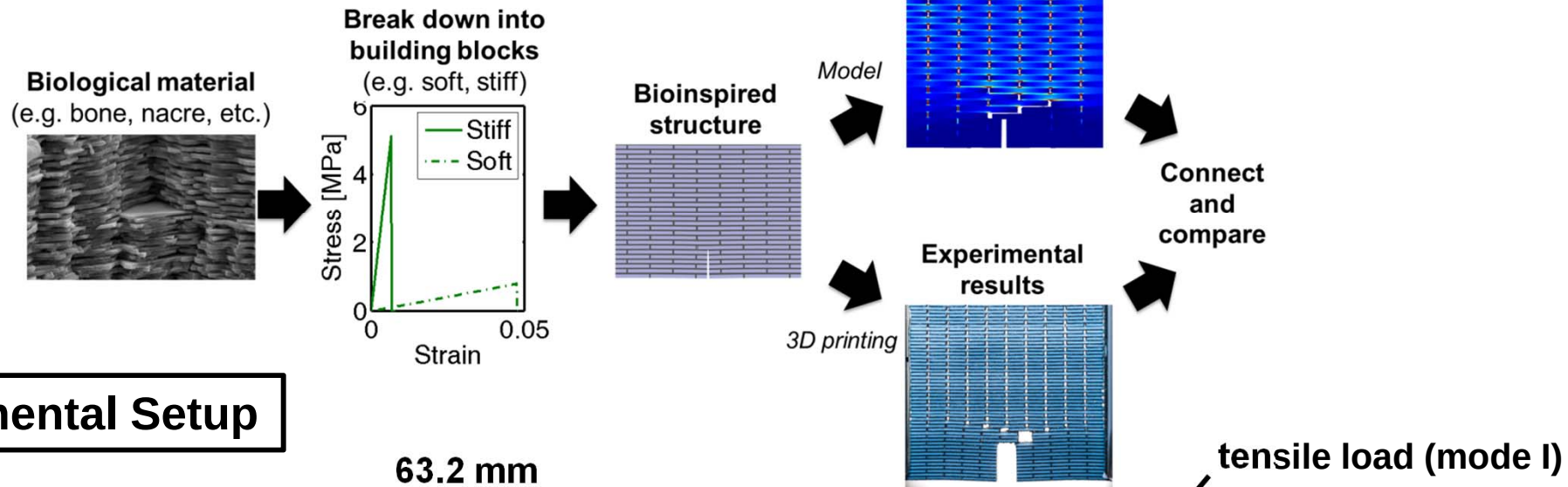
- Develop hierarchical materials that resist brittle fracture and redistributes loading energy towards dissipation in large volumes, in modeling and experiment using 3D printing

• Approach

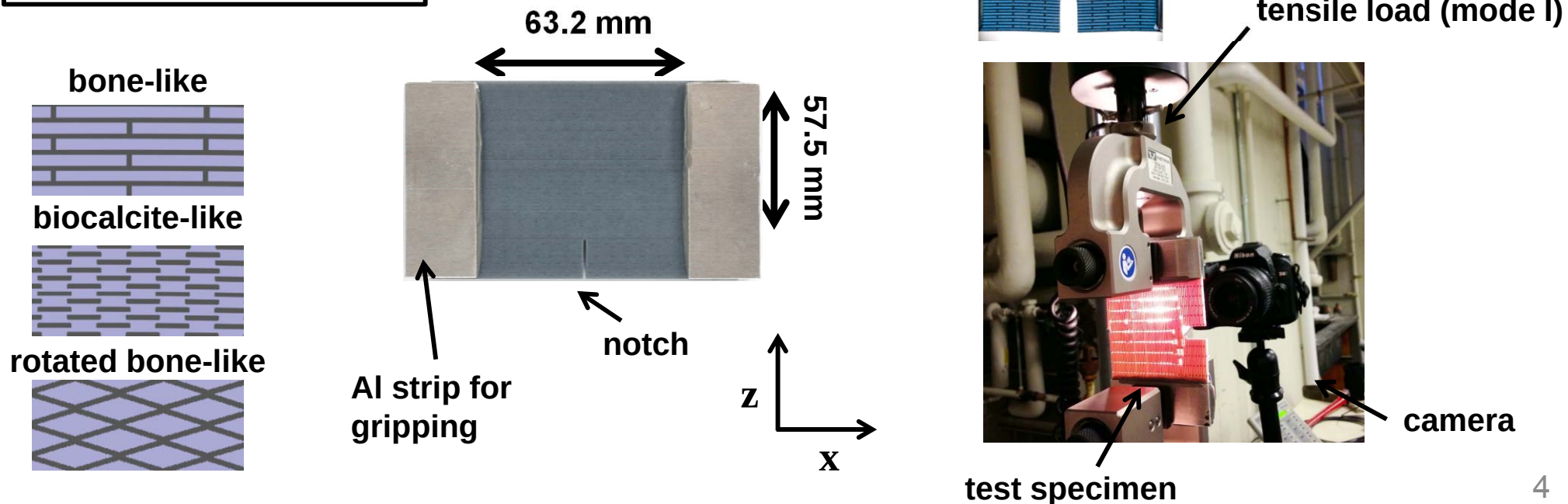
- Atomistic based, bottom-up multi-scale simulation combined with theoretical modeling, to quantify the **role of length-scales** and **material hierarchies**



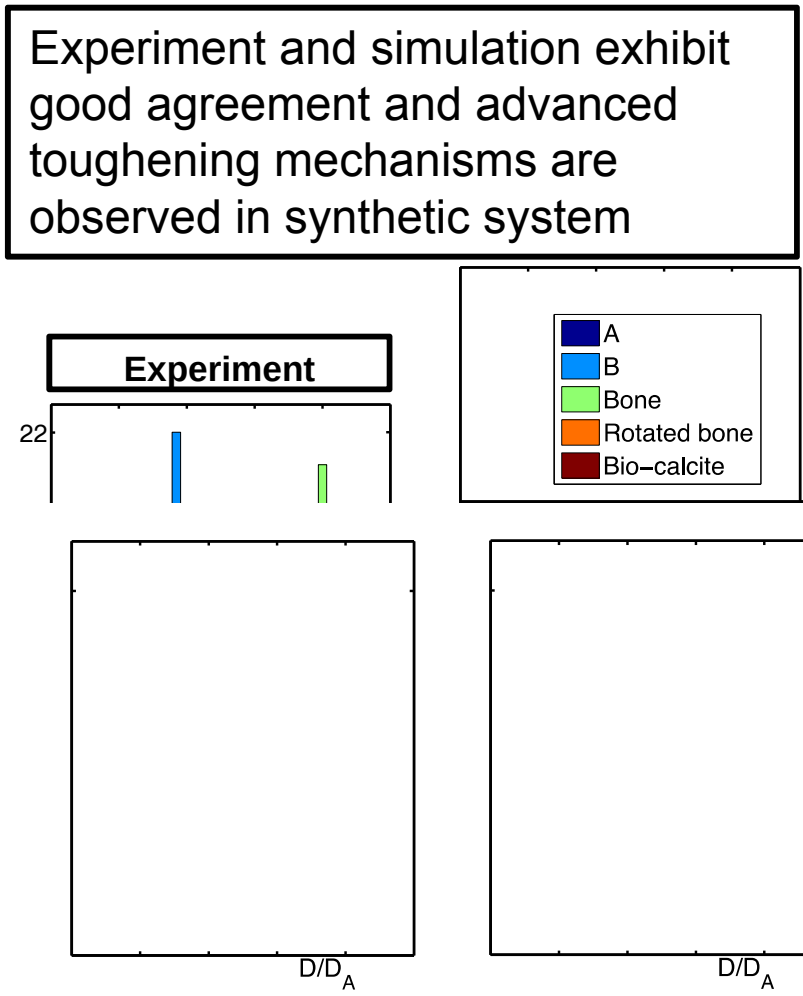
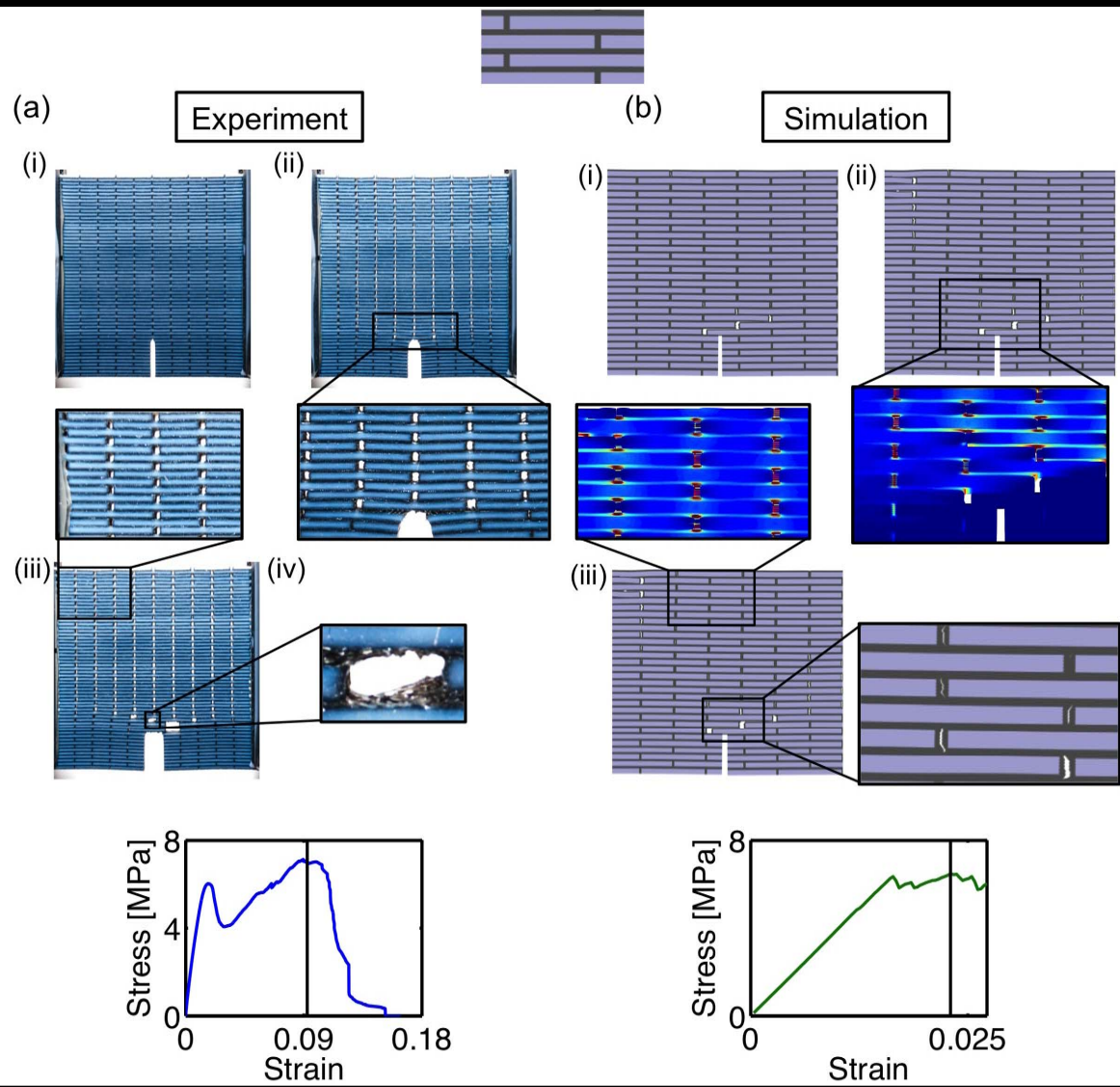
De-novo approach to design and synthesis



Experimental Setup



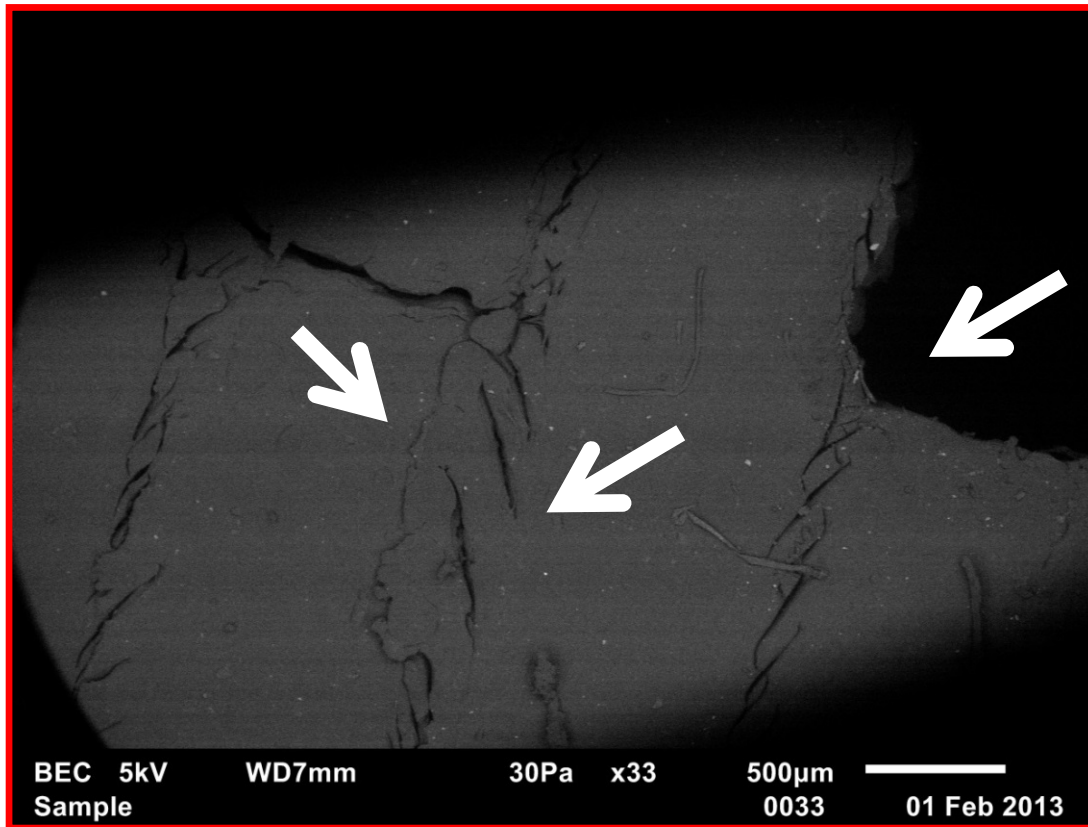
Markus Buehler, MIT, SI, \$282K, 36 Mo., 3rd year



3D printing of computationally designed hierarchical composites: SEM post fracture analysis

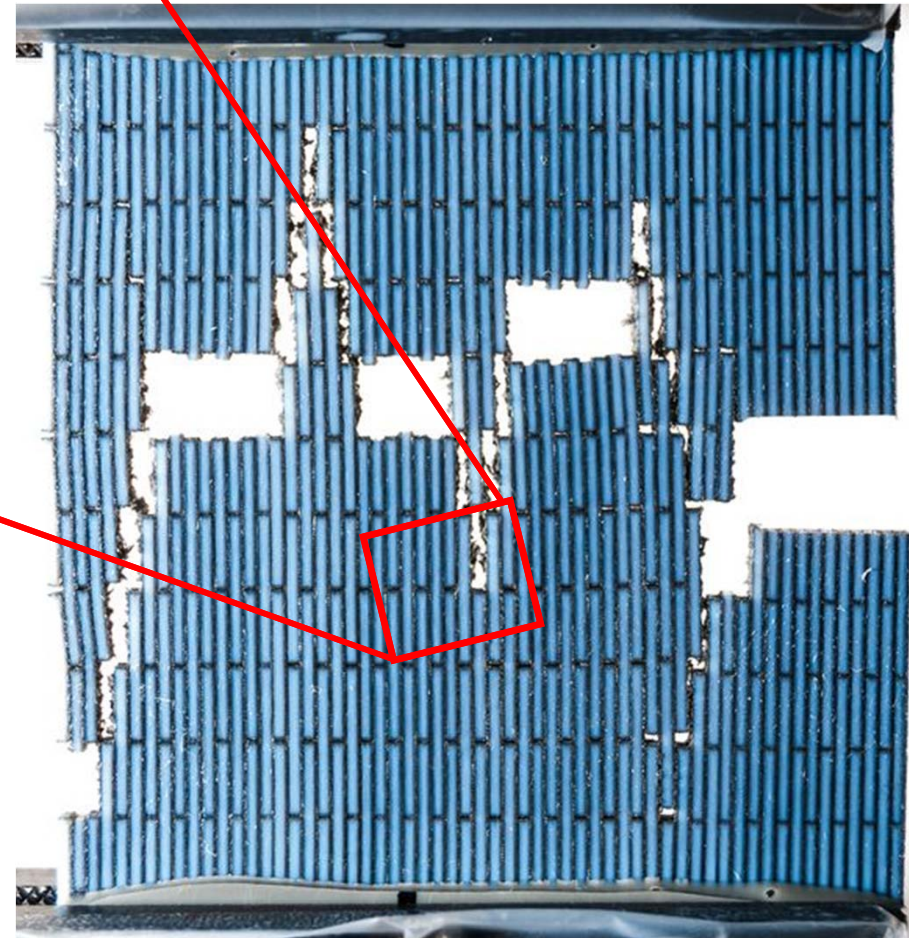
Solid Mechanics

Markus Buehler, MIT, SI, \$282K, 36 Mo., 3rd year



Left: Detailed SEM analysis at the microscale (example)

Bottom: Experimental imaging



- Samples confirm **distributed failure**
- **Strong interfaces** (NO interfacial debonding)
- **Increased fracture toughness** due to hierarchical architecture – long fracture path

Markus Buehler, MIT, SI, \$282K, 36 Mo., 3rd year

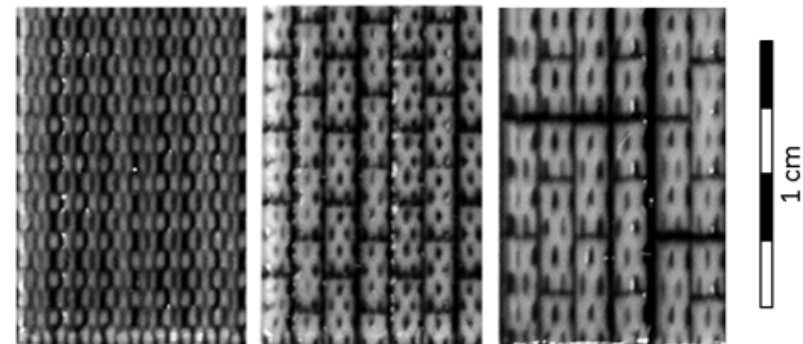
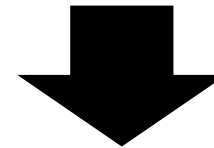
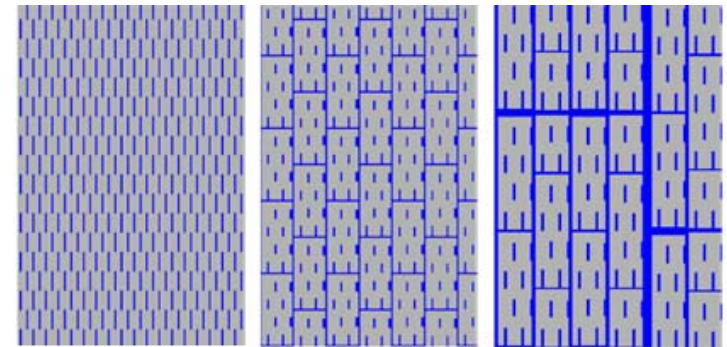
• Scientific Accomplishments

- This study identifies novel design mechanisms and demonstrates 3D printing as a means to create fracture resistant composites.
- Developed multiscale model to analyze the mechanics of materials with disordered mechanical properties
 - Developed framework has the potential for multiscale uncertainty quantification (UQ), could be combined with current model to improve predictions

▪ Army Impact

- A new paradigm of composite design and manufacturing using 3D printing will enable the next-generation of composites to design novel lightweight ultra-tough structural materials.

Computer model



**3D printed specimen (exact
replica of computational model)**

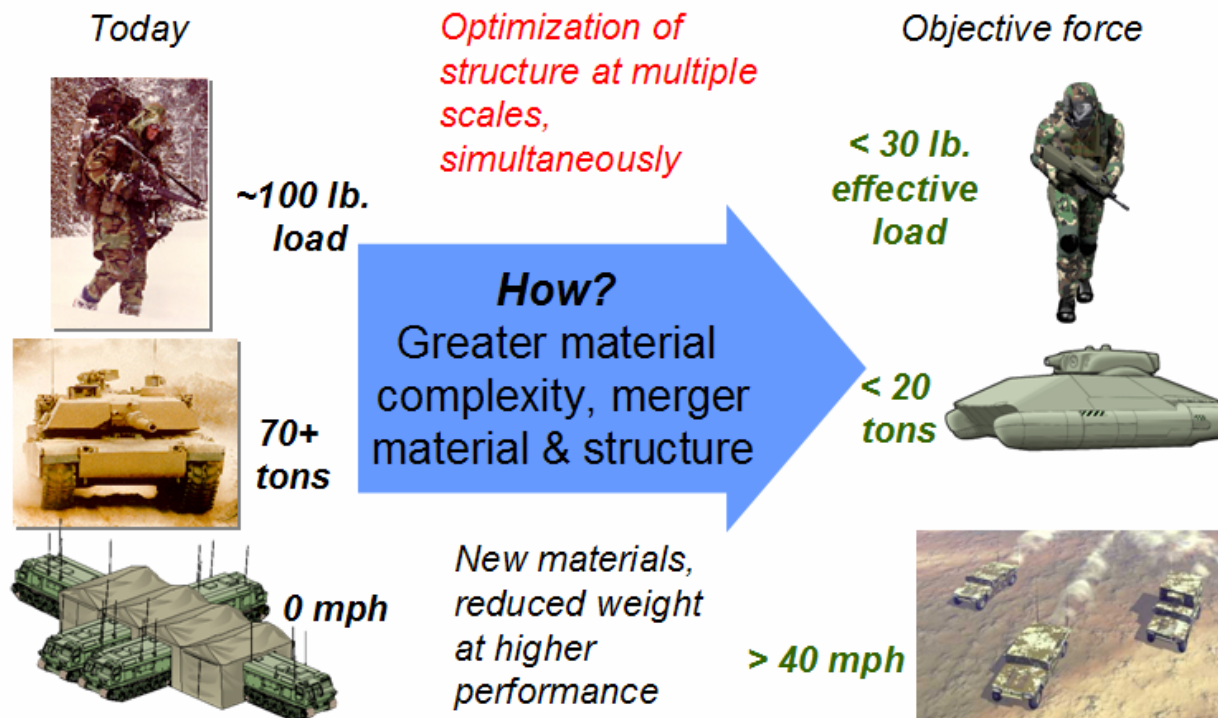
“Materials by design”

- Transitions
 - A discussion with Dr. **Jan Andzelm** at ARL is ongoing, focused on chemistry, materials, multiscale modeling and applications of collagen materials
 - **MURI project** funded (start date end of 2009), focused on the design of disruptive fibers and mats of carbon nanotubes
 - **Keynote/plenary speaker** at many conferences and workshops, enabled outreach to academic and technical community
 - Relevant for new **ISN project** with Raul Radovitzky (MIT): Develop lightweight armor materials/multiscale method development (complementary)
 - Talks given at **EDRC** (Drs. **Charles Cornwell**, **Mei Chandler**, and others); individuals from EDRC hosted at MIT for discussions
 - Started collaboration with Dr. **Stephen Bartolucci** at **US Army Benet Laboratories** (graphene-aluminum composites)
 - Teach **MIT Professional Education Program** in June 2012 (“Materials By Design”, geared towards industry (http://web.mit.edu/professional/short-programs/courses/materials_by_design.html))
 - Participation in ARO workshop “**Issues and Challenges in Nanomanufacturing, Additive Manufacturing, and Advanced Manufacturing**”, October 1-2, 2013: Alumni Center, North Carolina State University
- PI Awards
 - Received several major awards from key societies:
TMS Hardy Award, IEEE Holm Lecture, MRS OYI Award, Society of Engineering Science Young Investigator Medal 2012, promotions to Tenure at MIT (2011), and Full Professor in 2013, and others

Multi-scale hierarchical and topological design of structures for failure resistance

• Army Impact

- This work has **several mid-term and immediate impacts** for Army capabilities
- Results of this research will enable the **next-generation of composites**, and enable a new engineering paradigm to design of novel protective coatings, helmets or textiles.
- The work will also lead to **new lightweight ultra-tough structural materials**.
- New paradigm of composite design and manufacturing using 3D printing developed (**immediate impact**)



Demonstrates: MATERIALS BY DESIGN

We realized an approach by which we start by atomistic simulation, use coarse-graining and inverse methods, to come up with optimal designs that can be 3D printed. 3D printed specimens are tested and analyzed, and show improved fracture properties.