# Materials in Extreme Dynamic Environments

## A Collaborative Research Alliance

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*The Johns Hopkins University (LRO)*
*Recipient Program Manager*

**Dr. John H. Beatty**
*US Army Research Laboratory*
*Cooperative Agreement Manager*

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# What are "Extreme Dynamic Environments" ?

ARL


**Strain Rates up to $10^6$, Pressures up to 50 GPa**

# Outline

- Background for MEDE CRA & Goals
- Approach and Uniqueness
- Research Team and Program Structure
- Science of Materials in Extreme Dynamic Environments
- Technical Challenges and Activities by Material Class
- The Collaboration

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# Program Basis: Why MEDE

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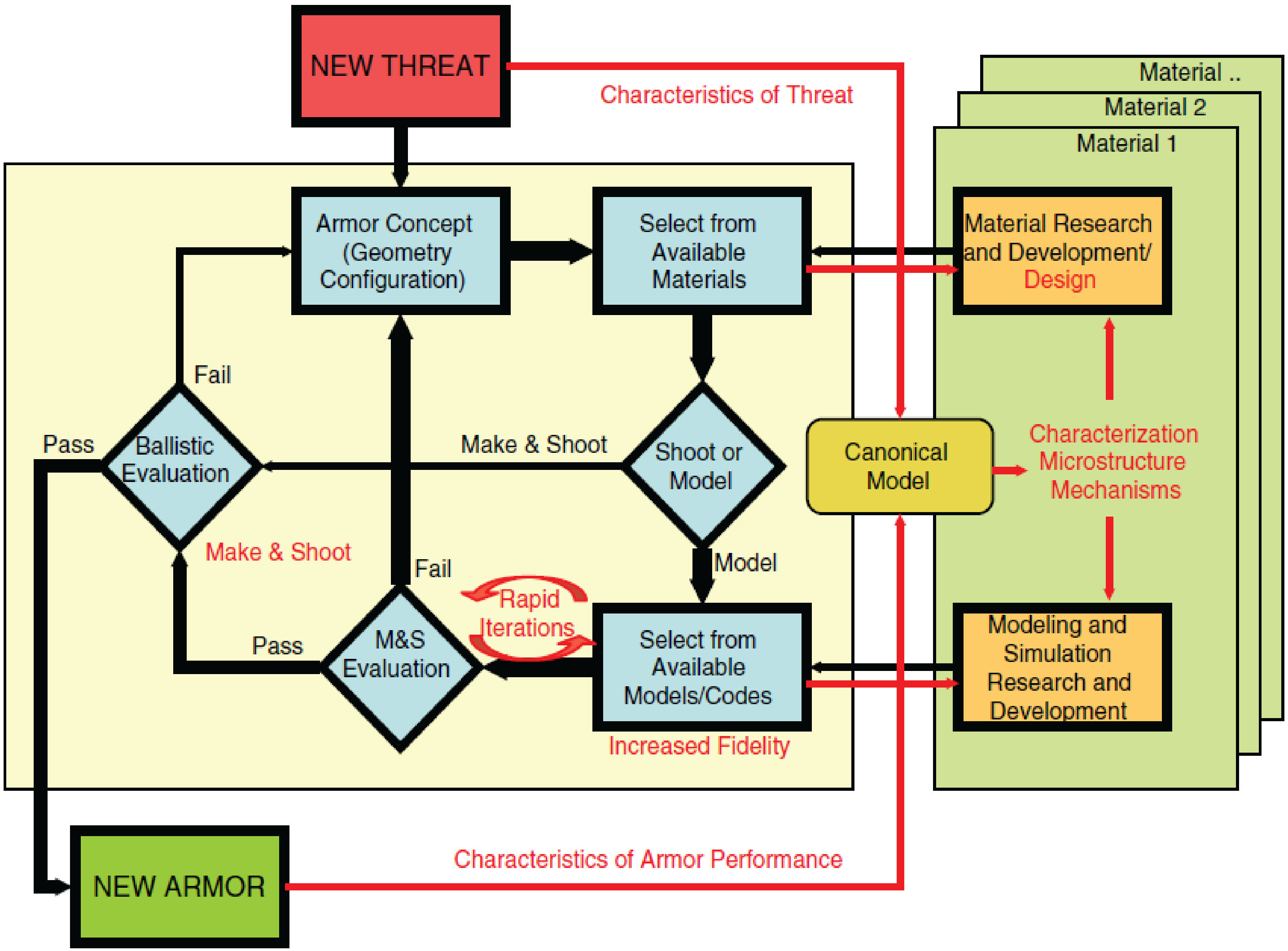
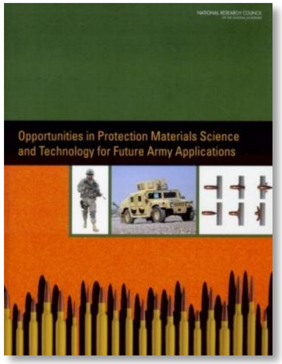


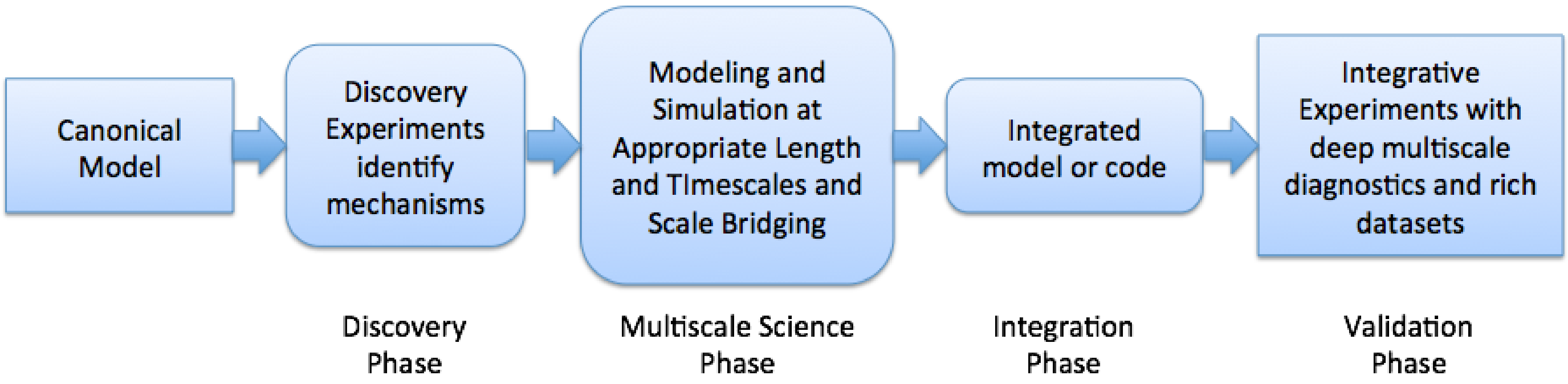




**From BAST/ NMAB report:**

**DoD should establish a defense initiative for *protection materials by design*…it should include a combination of computational, experimental, and materials testing, characterization, and processing research conducted by government, industry, and academia**

**FUTURE PAYOFF** **Vehicle and Soldier Protection - 1/3 savings in weight**

# MEDE Approach




## MEDE Uniqueness:

**Canonical model used to translate the application to basic science needs**

**Discovery phase is critical – we don't yet know property/performance trade-offs**

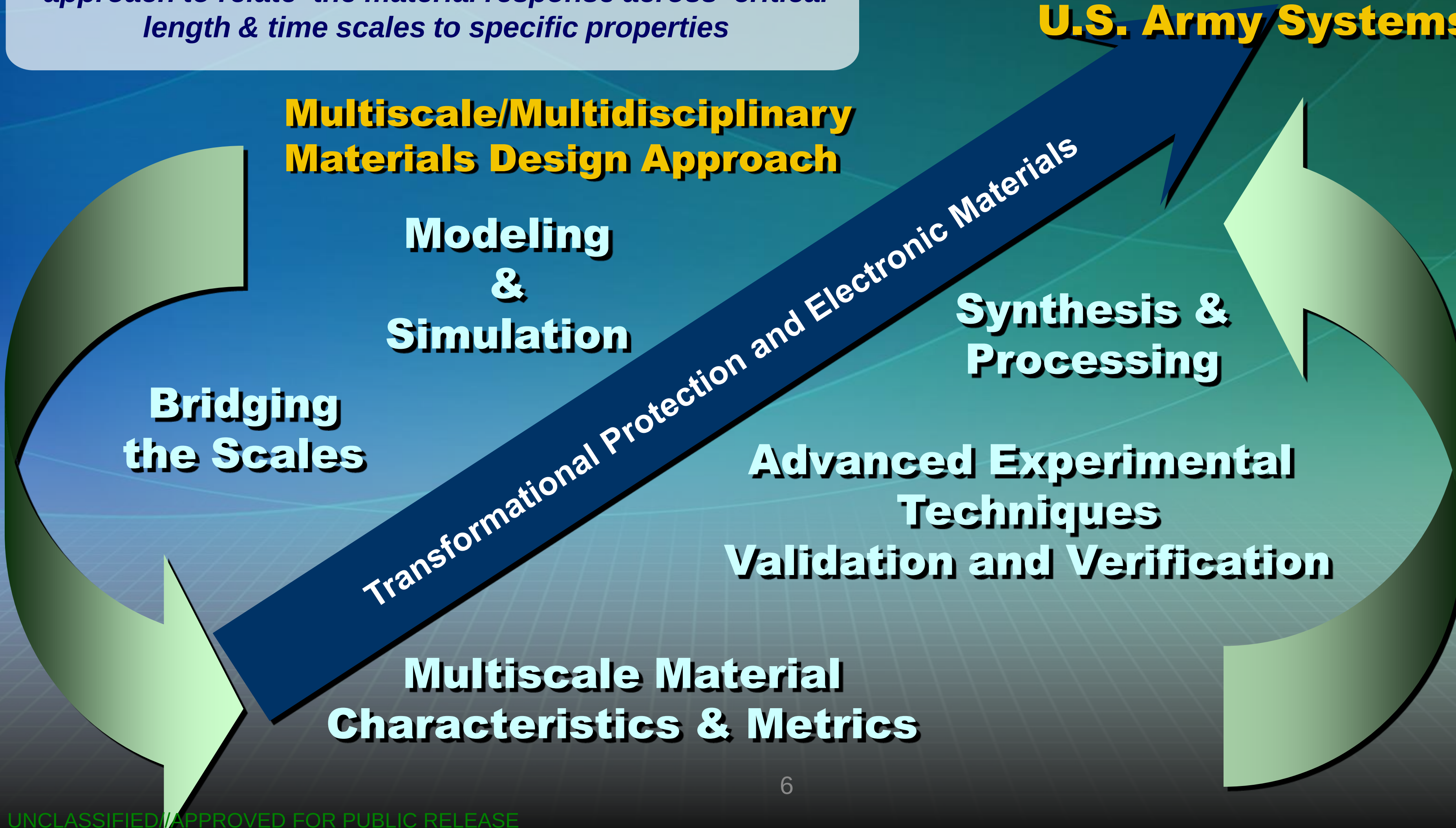
**Materials by design for protection materials**

# CRA Research Strategies

## Approach

*Fundamental research with a "materials by design" approach to relate the material response across critical length & time scales to specific properties*

## Protection and Electronic Materials for U.S. Army Systems



# Materials in Extreme Dynamic Environments (MEDE) Collaborative Alliance Members

## LRO: Johns Hopkins University

Program Director: K.T. Ramesh

Hopkins brings expertise in experiments under extreme conditions, characterization and modeling from atomistic to continuum scales, scale-bridging, and science-based parameterization

## Rutgers University

Principal: Richard A. Haber

Rutgers brings expertise in the processing and fundamental properties of ceramic materials, characterization and modeling at multiple scales, process modeling

## California Institute of Technology

Principal: Kaushik Bhattacharya

Caltech brings expertise in modeling across the scales, scalable computational methods, nanoscale and microscale experiments, and high strain rate characterization

## University of Delaware

Principal: John W. Gillespie, Jr.

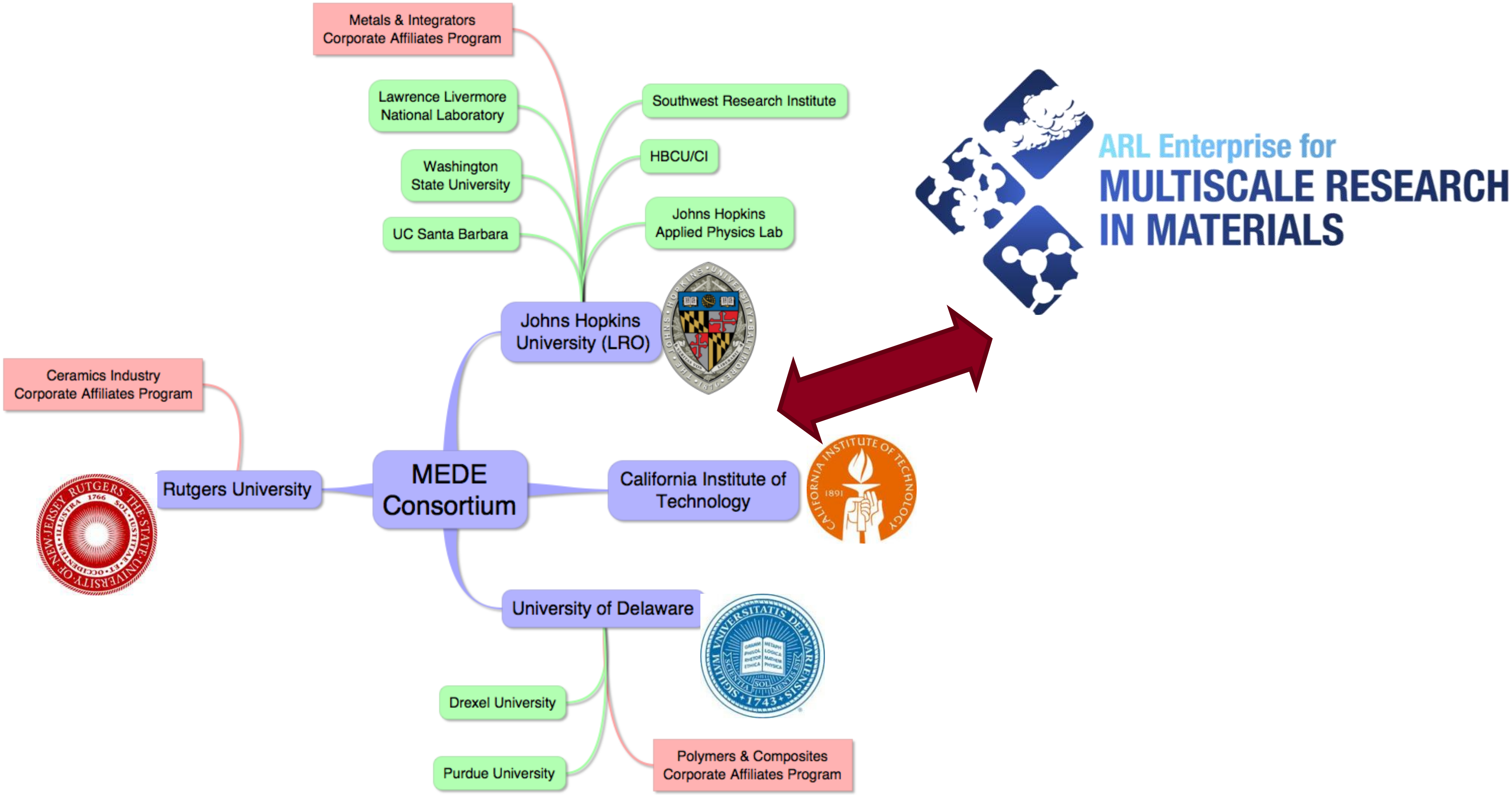
UDel brings expertise in polymers, the design, characterization and modeling of composites across multiple scales, processing of polymers and composites, interphase science

## US Army Research Laboratory

Collaborative Alliance Manager: John H. Beatty

ARL Brings expertise in armor design and armor materials, constitutive modeling, multiscale modeling, high strain rate characterization, computational tool development, transition

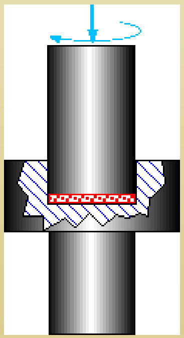
# MEDE CRA Institutions

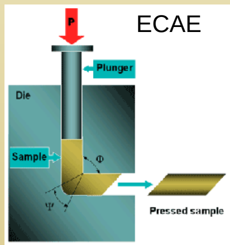



**Army-Academic-Industrial-National & Global Collaboration Engine**

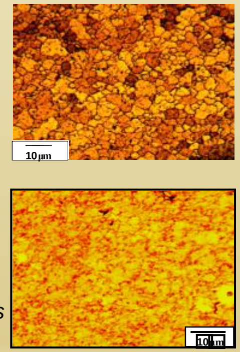
# Significant Efforts within ARL and the JHU MEDE Consortium

## Magnesium

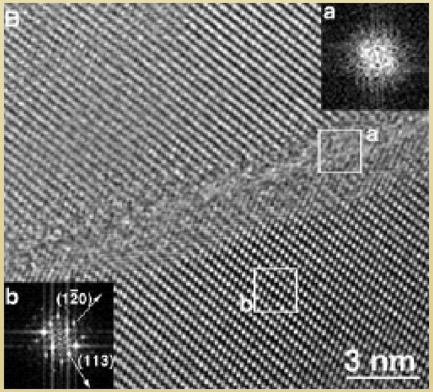




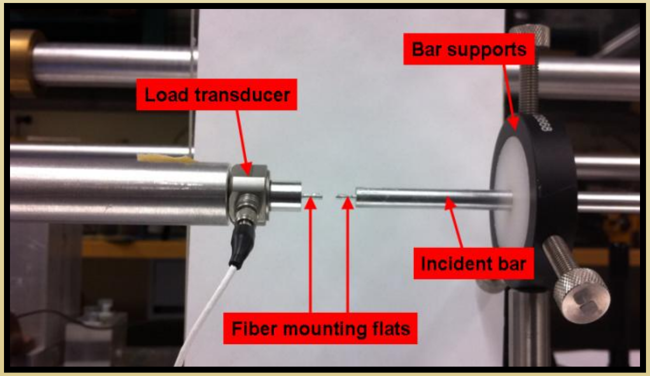

*Deformation Processing increases mechanical properties by reducing grain size.*




## Boron Carbide

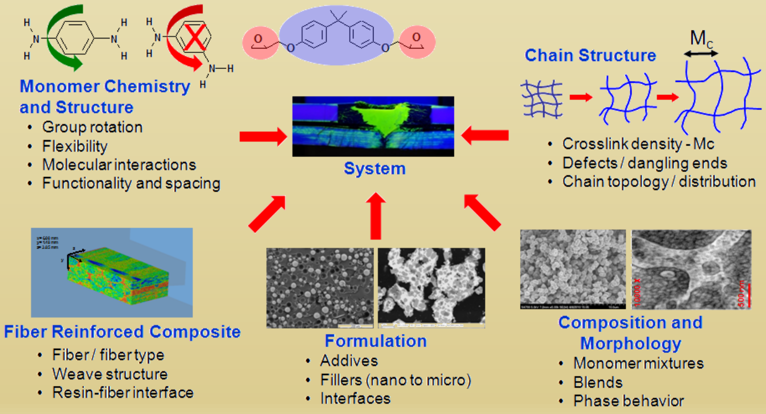



## Ultra-High Molecular Weight PolyEthylene




Unique High Loading-Rate Apparatus for Single-Fiber (~10 um diameter) Experiment

## S-Glass/Epoxy




**Mg, B4C, UHMWPE, S-Glass/Epoxy are important to future protection systems for Soldiers and Vehicles**

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# Technical Structure

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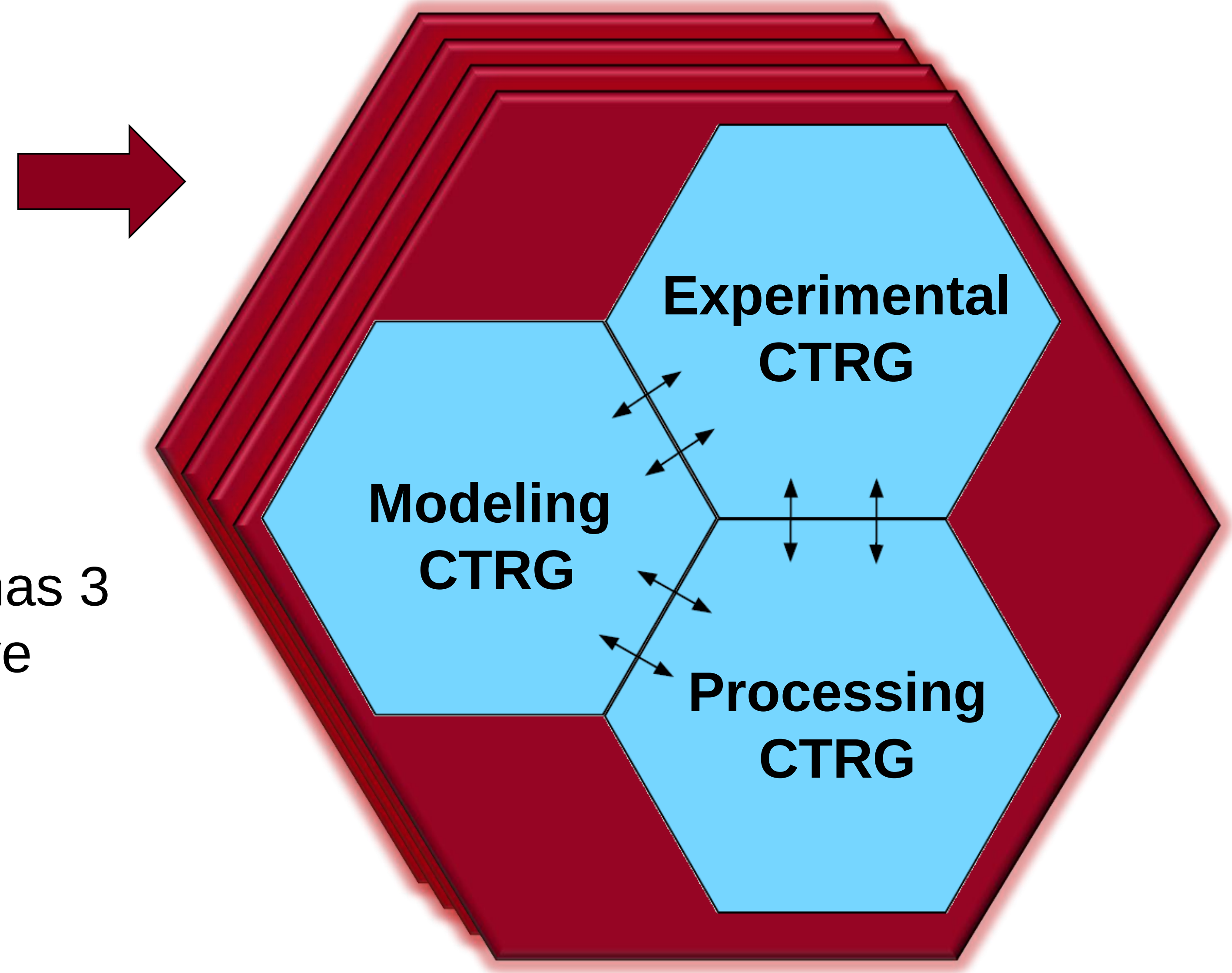
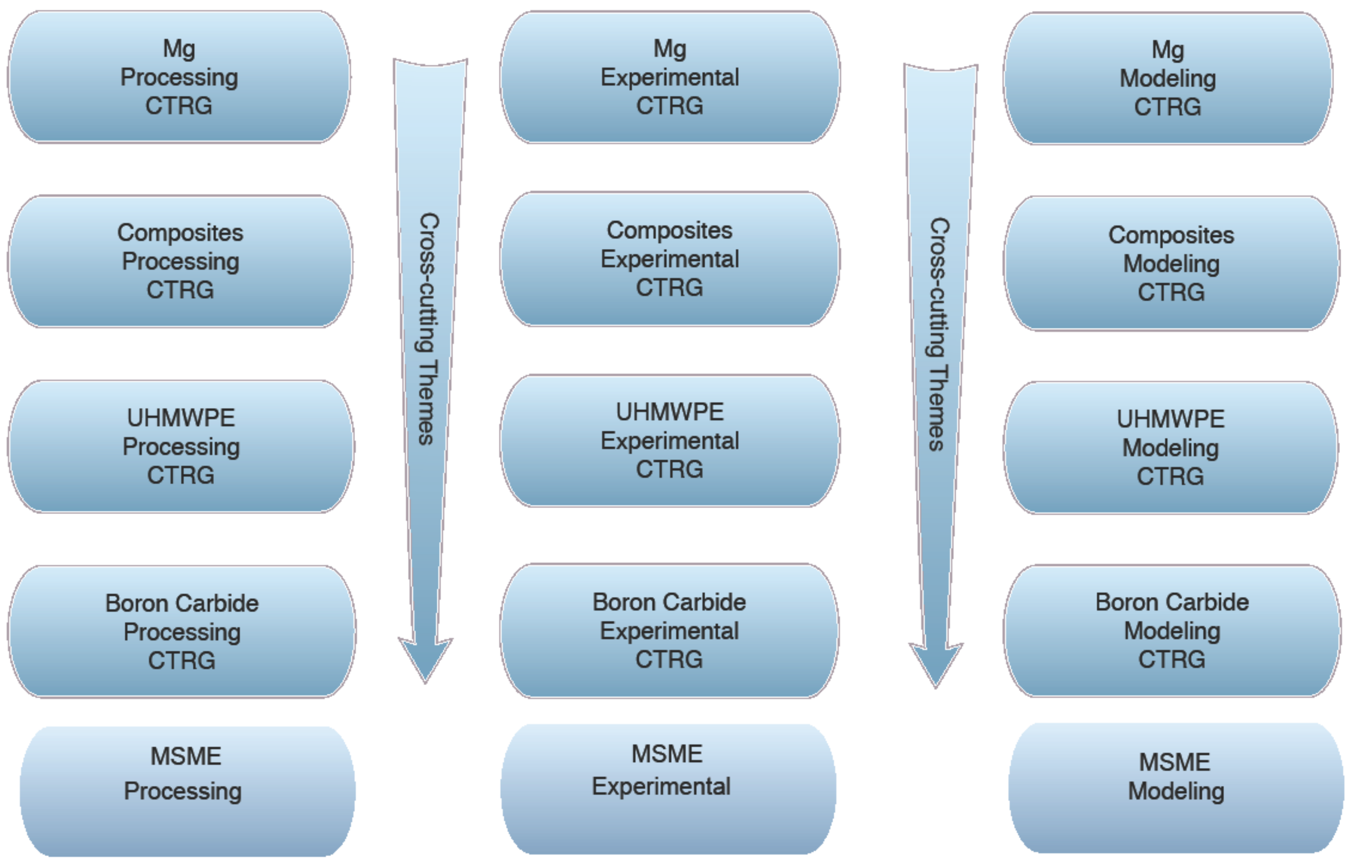
4 Materials Collaborative Materials Research Groups (CMRGs)

Each CMRG has 3 Collaborative Technical Research Groups (CTRGs)

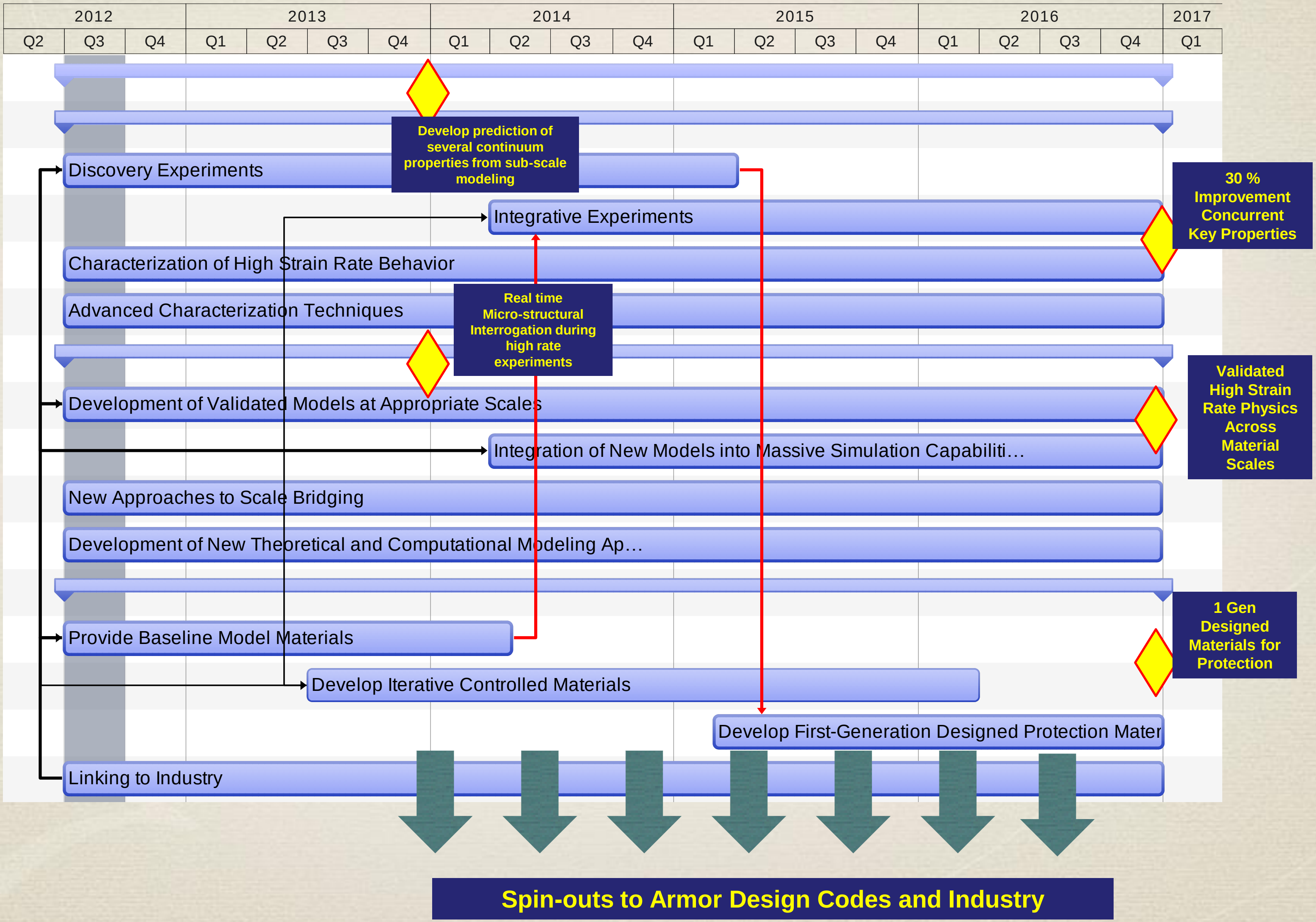


# Tasks Organized by Material

# Collaboration by Cross-cutting Themes



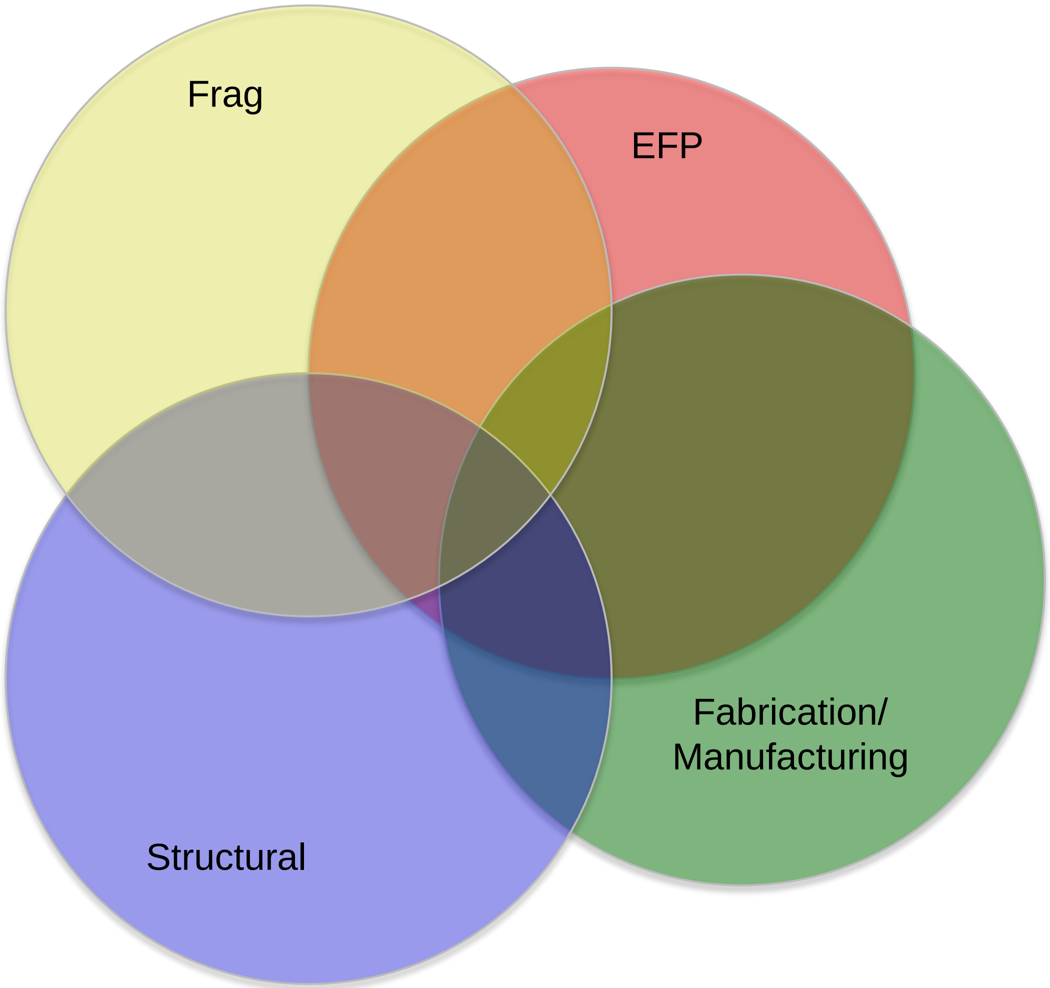
# MEDE CRA Schedule



# An Overview of the Science of MEDE

- Conceptual approach (design constraints)
- The science of extreme dynamic events
- The mechanism-based Materials by Design strategy for Materials in Extreme Dynamic Environments
- State of the art for each material system
- Collaborative approaches for each material system

# Conceptual Approach to the Design of Protective Materials for Extreme Dynamic Environments



# Science of Extreme Dynamic Events: Mechanisms

- Extreme dynamic events (e.g. terminal ballistics) involve deposition of large amounts of energy in very short times
- The speeds at which energy can propagate away from point of deposition are finite (wave speeds, crack speeds)
- As a result, the local energy density rises very rapidly, and the material seeks new internal pathways to dissipate this energy
- We call these energy pathways “mechanisms.”
- Which pathways (mechanisms) are available and are then expressed depends on the material and on the severity of the threat

# Mechanisms in Extreme Dynamic Events

- Dynamic deformation and failure *mechanisms* (not just material properties) dominate extreme dynamic events
- What are the mechanisms? Have to be able to see them *during* the extreme event.
- Each combination of material and threat leads to a specific spectrum of dynamic mechanisms.
- To *control* response to extreme event, we must control the mechanisms.
- To *design* the material for performance in the extreme event, we must *design* the expression of that mechanism spectrum.

# A Mechanism-Based Materials by Design Strategy for MEDE

- See it.
  EXPERIMENTAL CTRG
- Understand it.
  MODELING CTRG
- Control it.
  PROCESSING CTRG

→ ***Design* it.**

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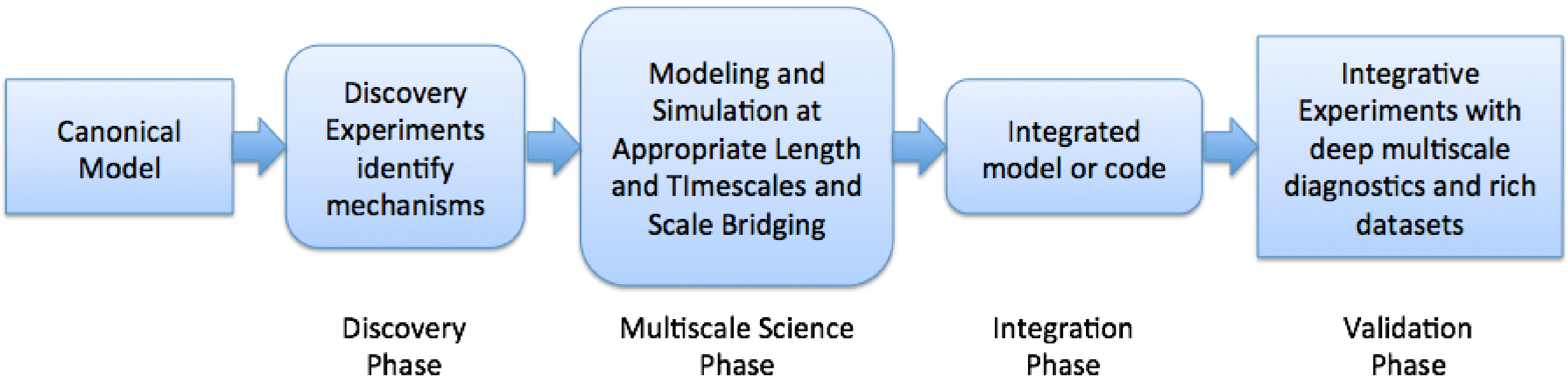
# The Science of Extreme Dynamic Events: Scales

- As the local energy density increases, the energy dissipation in the system must explore smaller and smaller length scales
- For example, such an analysis suggests that many blast problems can be addressed through mm-scale structural control
- However, for ballistic problems we must design and control energy pathways at the micron-scale.
- Micron-scale dynamic mechanisms are very strongly dependent on nanoscale and atomistic behaviors at very short times.
- The extreme dynamic environment typically exercises the full range of length scales and timescales, making this the quintessential multiscale problem.

# Multiscale Modeling Strategy for MEDE




Clearly identify “discovery experiments” and “integrative experiments” in EDE

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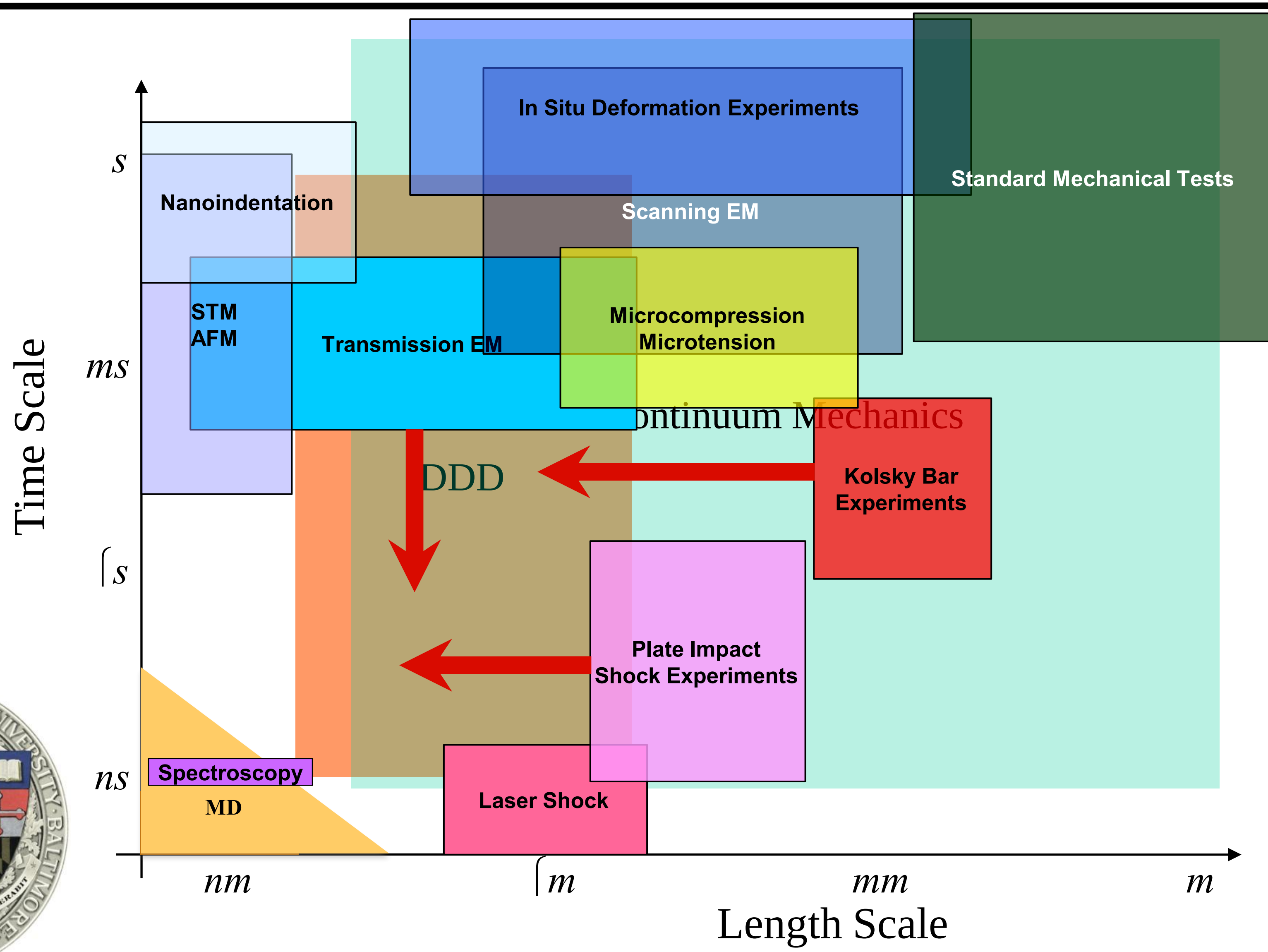
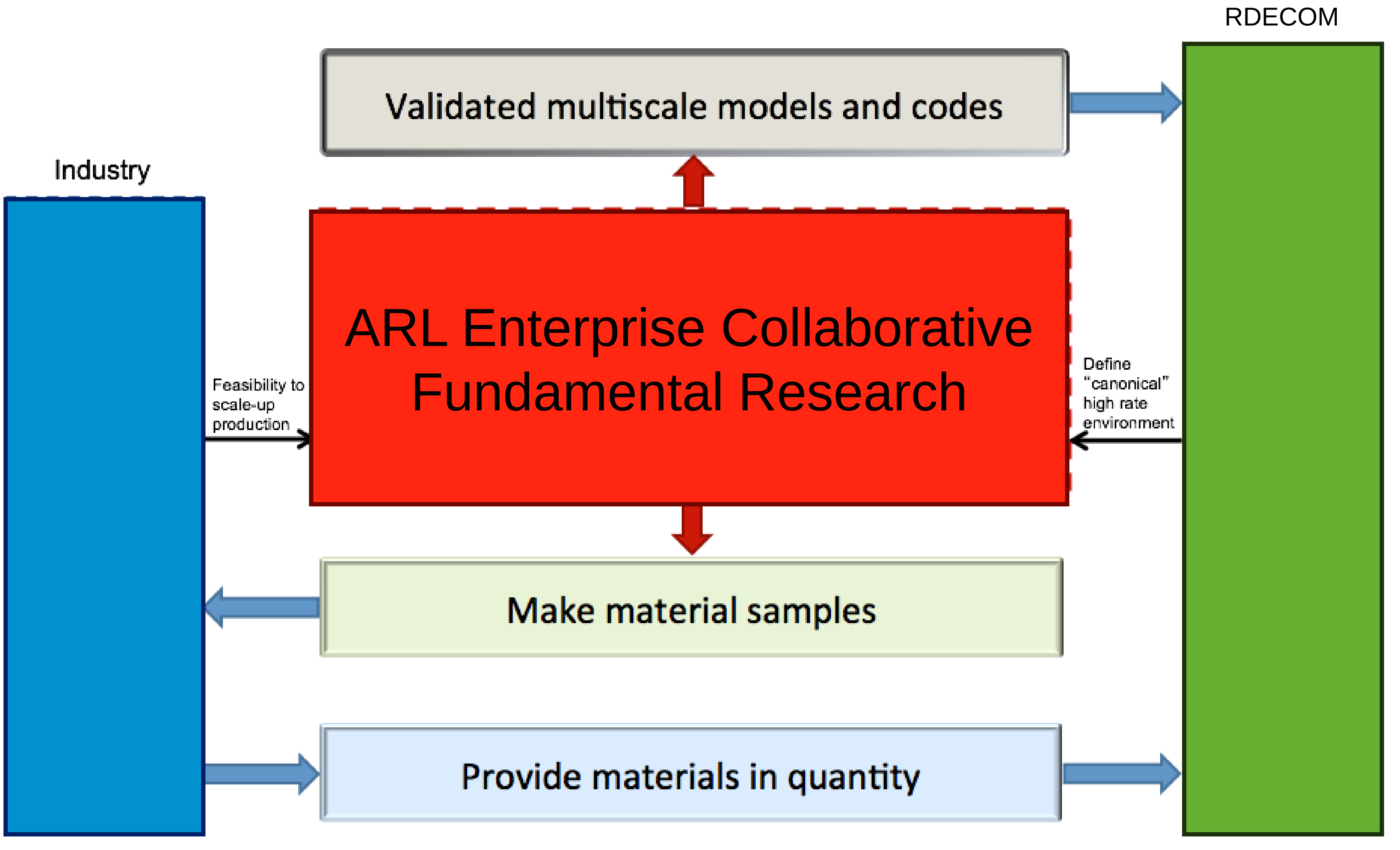
# Expanding the Domains of Validity of Current Experiments and Modeling



# Global Multiscale Materials by Design Strategy



# What is the State of the Art?

# State of the Art for Metals (Magnesium)

| Scale or Technical Core Element | Primary Mechanism | Advanced Exper. Tech. -1- | Modeling & Simulation -2- | Bridging the Scales -3- | Material Char. & Prop -4- | Synthesis & Processing -5- |
|---|---|---|---|---|---|---|
| **Atomic -a-** | *Electronic structure, thermal motion of nuclei, reactivity* | Spectroscopy, Shock Hugoniot, EELS | QM, DFT, MD, EAM | Coarse-grained DFT | Moduli, bond energy, $\gamma$-surfaces, core energies, SFE, EoS | Chemistry, alloying |
| **Crystal -b-** | *Dislocation cores, slip & interactions (hardening), dislocation density evolution and patterning, twinning, thermal softening, phase transformations* | HREM, TEM, Dynamic TEM, Kolsky bar, nanoindentation, microcompression, microtension, in situ X-ray diffraction, pyrometry | MD, discrete dislocation dynamics, discrete twinning dynamics, crystal plasticity, FEM | Hot QC, hyperdynamics | Subgrain and cell structure, inclusions, precipitates and dispersions, twin volume fractions, high rate behaviors | Dispersion and precipitation hardening, nano-composites |
| **Mesoscale -c-** | *Grain boundaries, grain and subgrain rotation, texturing, misorientation distribution, crack nucleation* | HREM, TEM, Dynamic TEM, Kolsky bar, X-ray microdiffraction, pyrometry | Crystal plasticity, gradient terms, Lagrangian (FEM, OTM), Eulerian (CTH) | Defect dynamics | Grain size distribution, grain morphology, texture, orientation distribution, high rate behaviors | Grain size control, grain boundary control, microstructural design |
| **Macroscale -d-** | *Anisotropic viscoplasticity, texture evolution, shear localization, massive fragmentation, spallation* | Shock expts, Kolsky bar, in situ microcompression, spall experiments, torsional Kolsky bar, expanding ring, pyrometry | Viscoplasticity, Lagrangian (FEM, OTM), Uncertainty Quantification, Eulerian (CTH) | Enhanced continua, nonlocal models, defect dynamics | High-strain-rate, high-pressure and high-temperature response, EoS, post-test damage assessment | Casting, rolling, extrusion, forging, ECAP/SPD |



| | | | | |
|---|---|---|---|---|
| Generally identified, understood or implemented | Sometimes identified, some understanding, some implementation | Weak identification understanding, or implementation | Poorly identified, poorly understood, or early implementations | Not identified, not understood or not implemented |

# Magnesium: A Model Metal System

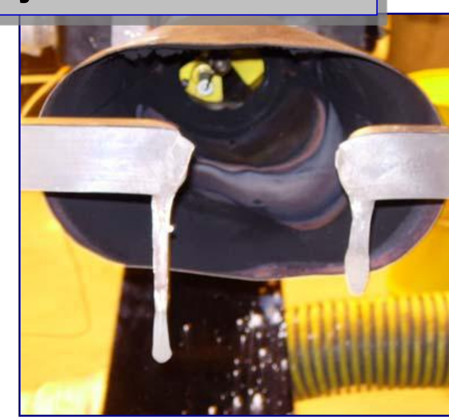
- Magnesium has the lowest-density of the structural metals
- One of the most abundant metals in the Earth's crust
- Density of 1.7 gm/cc - less than a quarter that of steel
- Primary difficulties are low strength and anisotropy
- Most rapidly growing metals industry (but small)

**Non-flammable Mg Stryker Troop Ramp Door**

**WE43-T5 alloy: Met all requirements, saved 127 lbs.**

**Next Generation of Mg Alloys are flame resistant.**

*AZ31 Mg alloy*
*Sample Burns After Melting*



*WE43 / ELEKTRON 21*
*No Burning After Melting*

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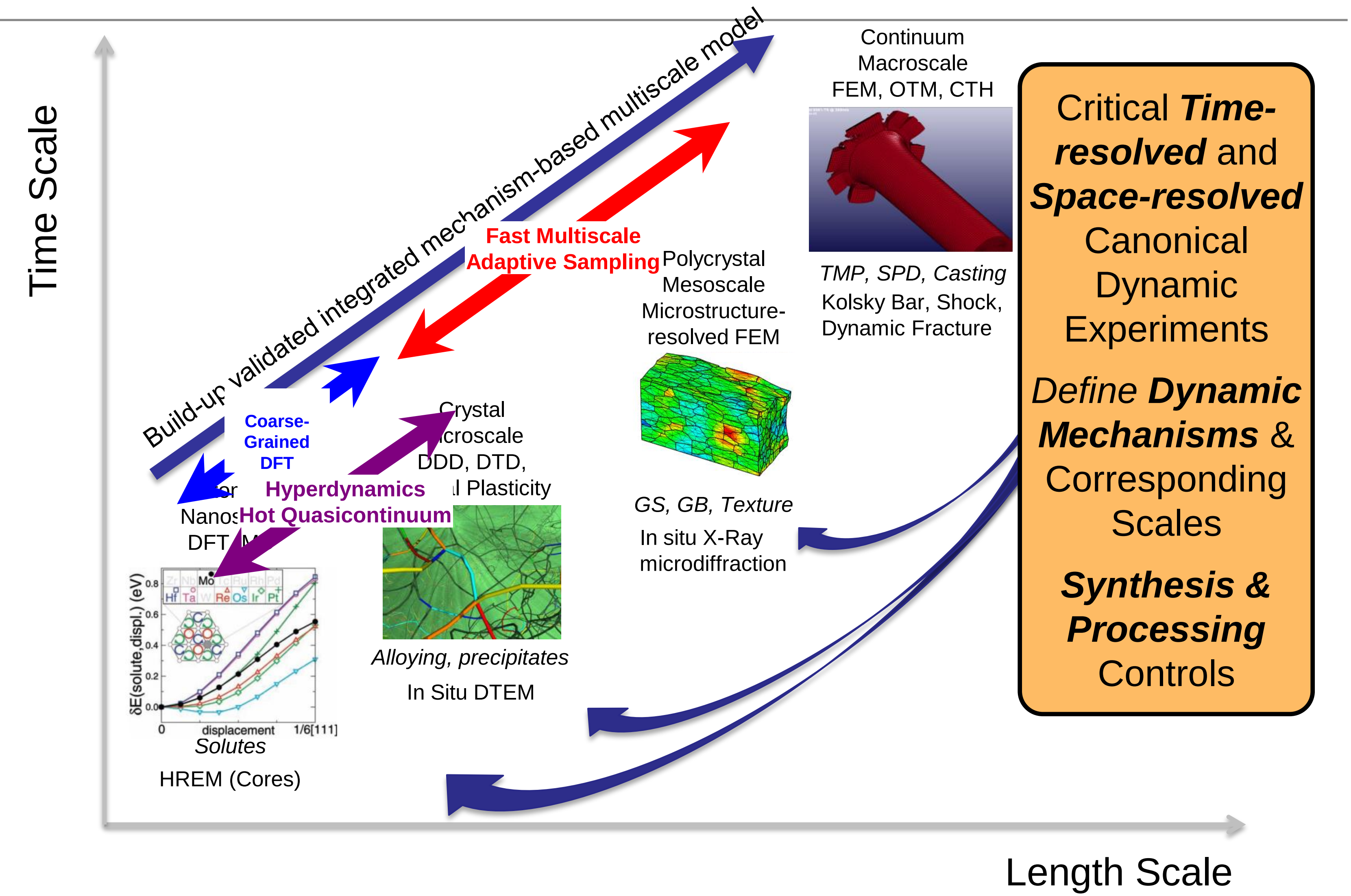
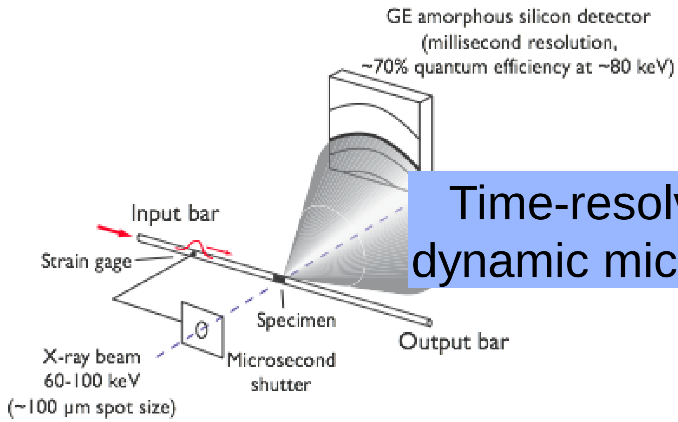
# MEDE Multiscale Strategy for Magnesium

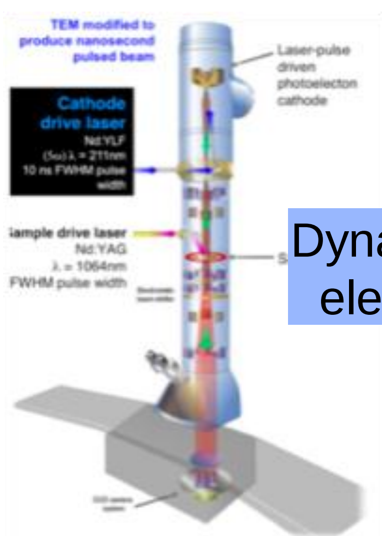


# Magnesium: Experiments and Characterization

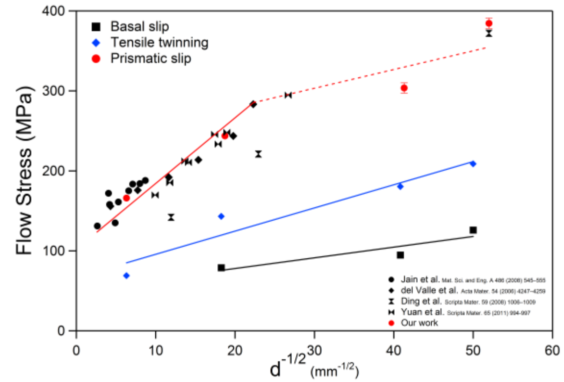
## Discovery Experiments




Time-resolved in situ dynamic microdiffraction

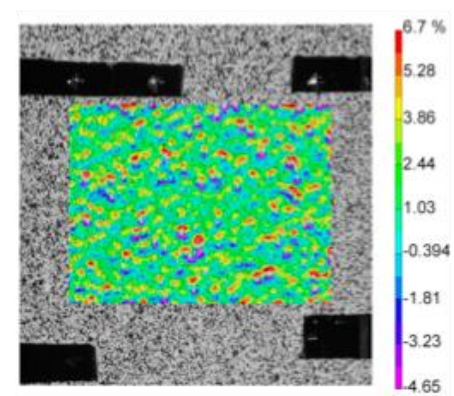



Dynamic transmission electron microscopy



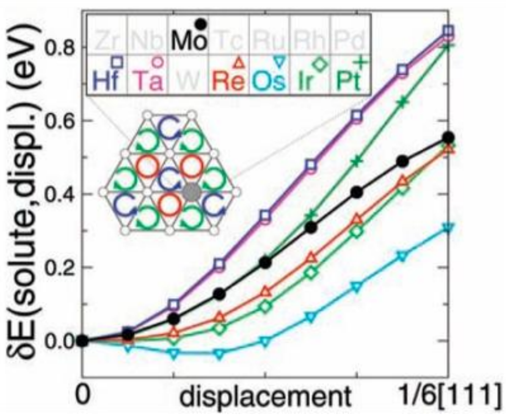

*Grain size hardening of prismatic slip and tensile twinning is very pronounced, whereas basal slip shows only small hardening.*

## Integrative Experiments

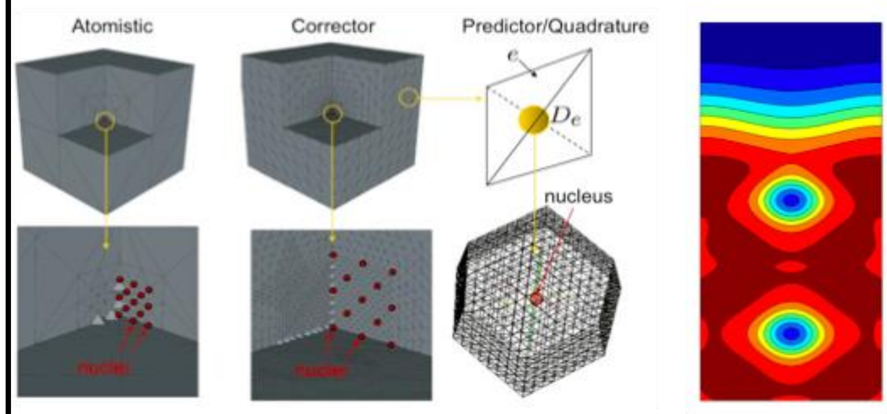



# Magnesium: Modeling and Scale-Bridging

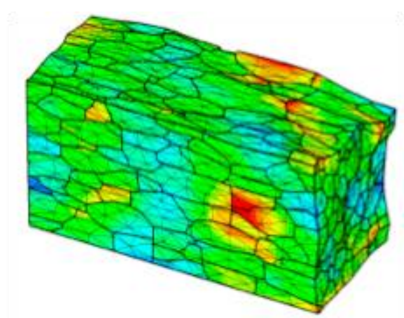
## Influence of Solutes on g-surfaces



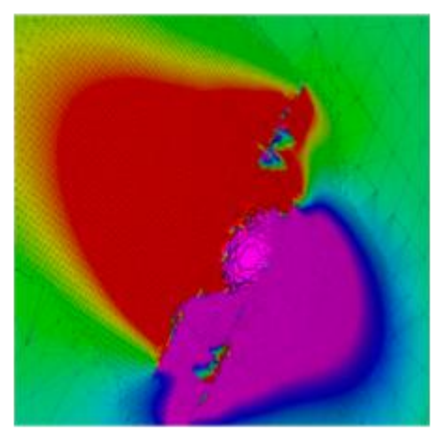

## Coarse-grained Density Functional Theory

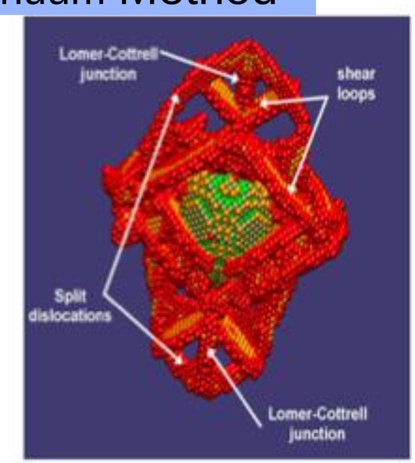



## Undeformed and deformed polycrystalline microstructures

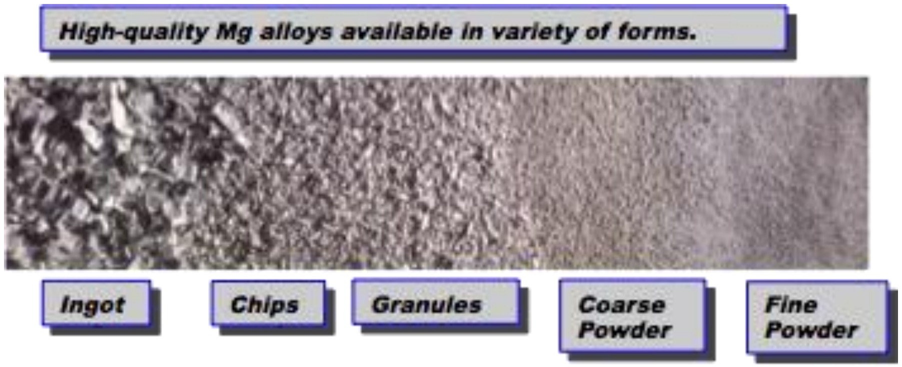


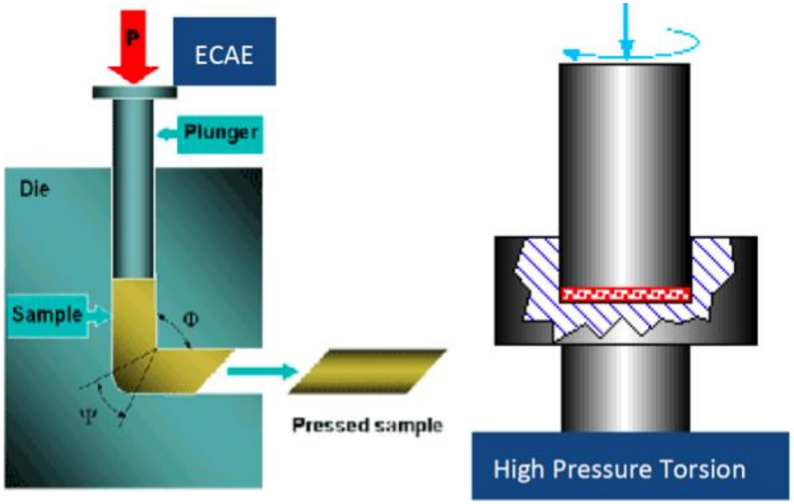
## The Quasicontinuum Method

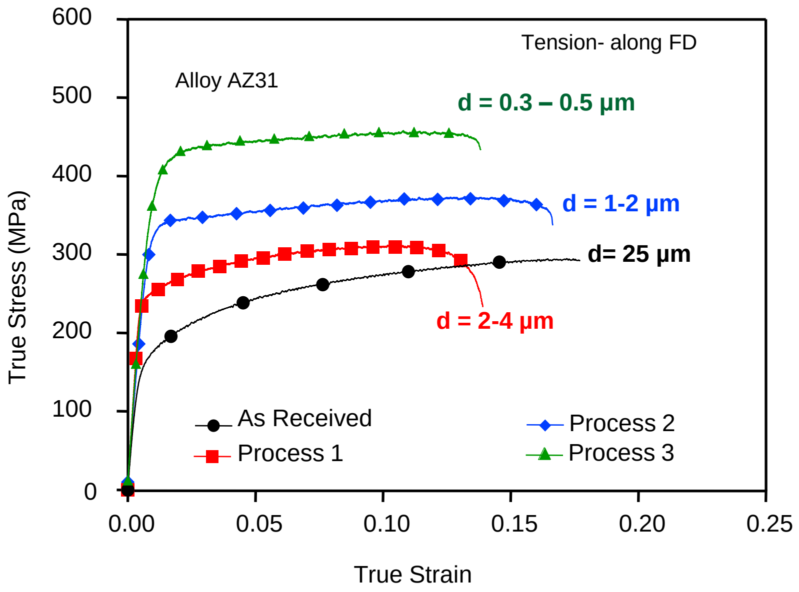


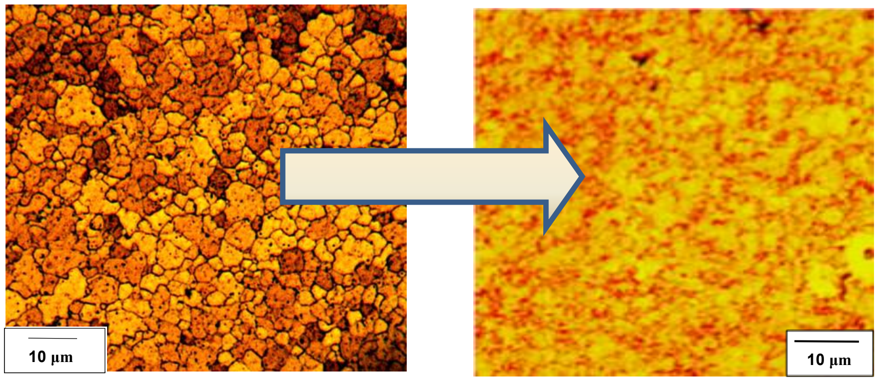


# Magnesium: Synthesis and Processing



# Boron Carbide: A Model Ceramic System

- Boron carbide is the armor ceramic with the greatest potential for revolutionary improvements
- The material has high hardness, and a high Hugoniot Elastic Limit
- Has a low theoretical density (30% less than that of SiC)
- However, it shows a pronounced loss of strength at high impact velocities


# State of the Art for Ceramics (Boron Carbide)

| Scale or Technical Core Element | Primary Mechanism | Advanced Exper. Tech. -1- | Modeling & Simulation -2- | Bridging the Scales -3- | Material Char. & Prop -4- | Synthesis & Processing -5- |
|---|---|---|---|---|---|---|
| **Atomic -a-** | *Electronic structure, thermal motion of nuclei, bond rupture* | Spectroscopy, Shock Hugoniot | QM, DFT, EoS | Coarse-grained DFT, potentials | Moduli, bandgap | Chemistry |
| **Crystal -b-** | *Cleavage, Amorphization, Twinning, Dislocation motion, stacking fault nucleation, twin-induced cracking* | HREM, TEM, Dynamic TEM, Kolsky bar, microcompression, nanoindentation, DAC | MD, discrete dislocation dynamics, discrete twinning dynamics, crystal plasticity | Coarse-grained DFT, hot QC, hyperdynamics | Anisotropic moduli, cleavage and twinning planes, intrinsic toughness | Powder production and control |
| **Mesoscale -c-** | *Triple-junction crack nucleation, Grain boundary failure, defect activated cracks, intergranular vs. transgranular fracture, crack interactions, anisotropic elastic effects on residual stresses and cracking* | HREM, TEM, Dynamic TEM, Kolsky bar, X-ray microdiffraction, instrumented indentation, phase contrast, in situ microcompression for GB strength, acoustic spectroscopy | Crystal plasticity, gradient terms, microstructure-resolved FEM and OTM | Defect dynamics, probabilistic models | Grain size distribution, grain morphology, texture, damage characterization | Grain size control, grain boundary control, microstructural design, advanced processing techniques |
| **Macroscale -d-** | *Fast crack growth, effective plasticity, anisotropic damage growth, short vs long cracks, texture, fragmentation* | Shock expts, Kolsky bar, spall experiments, in situ visualization of damage | Viscoplasticity, FEM, OTM, Uncertainty Quantification | Enhanced continua, nonlocal models, defect dynamics | High-strain-rate and high-pressure response, non-proportional loading, damage characterization | Sintering, hot-pressing, advanced processing techniques |

| | | | | |
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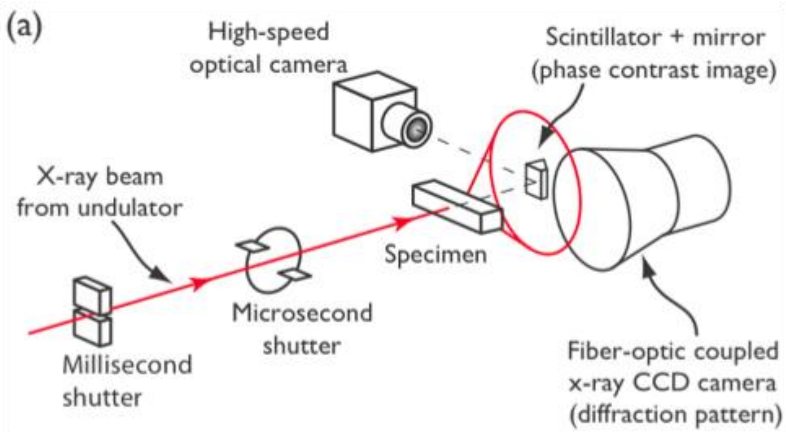
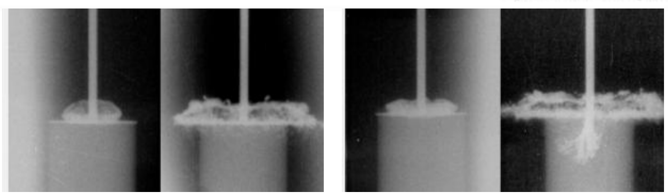
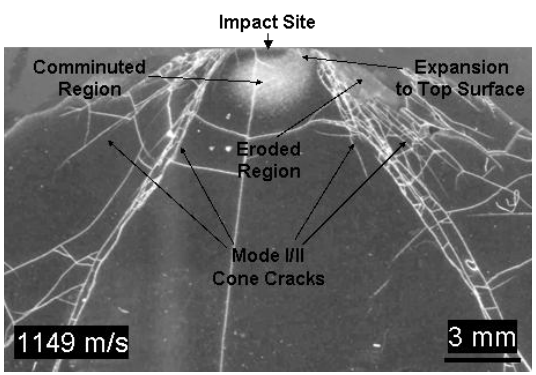
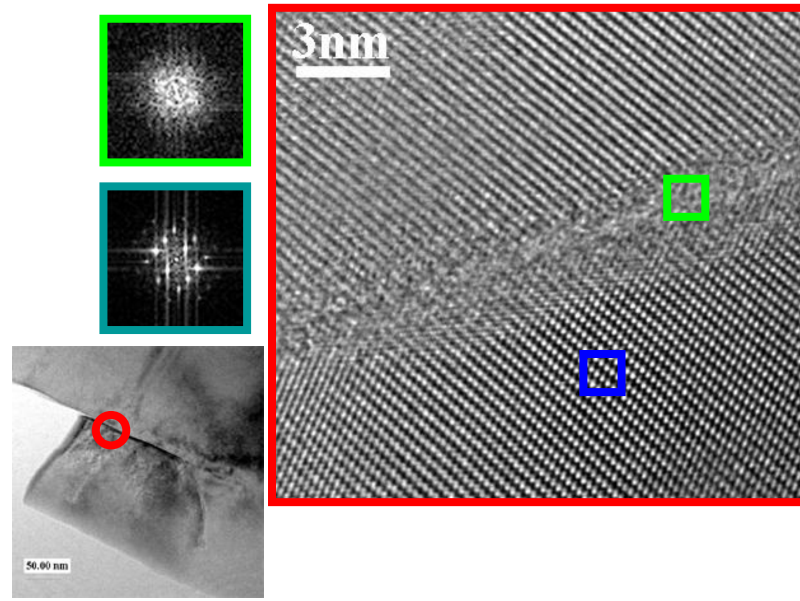
# Boron Carbide: Experiments and Characterization

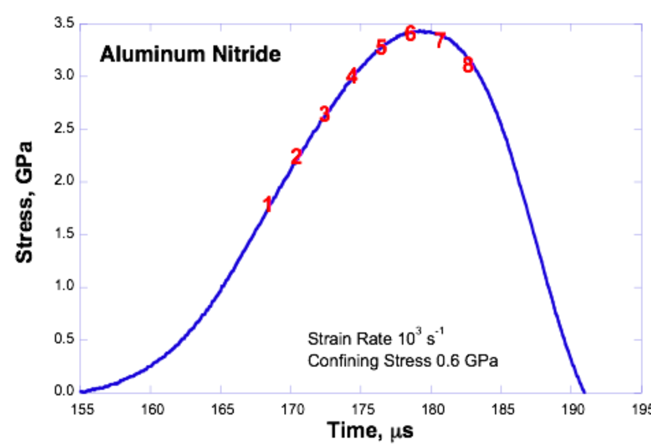
## Discovery Experiments

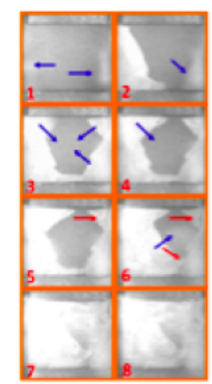




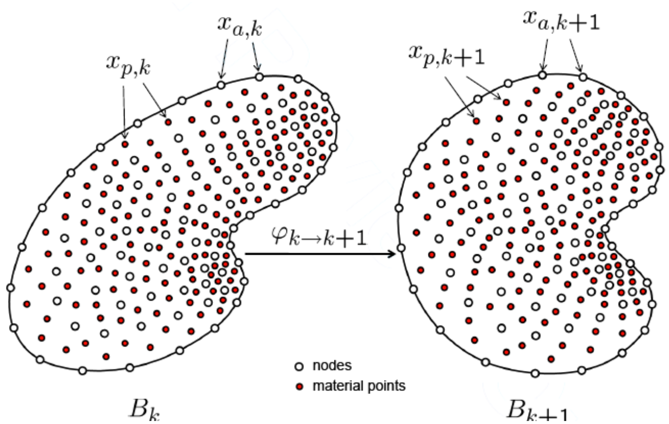



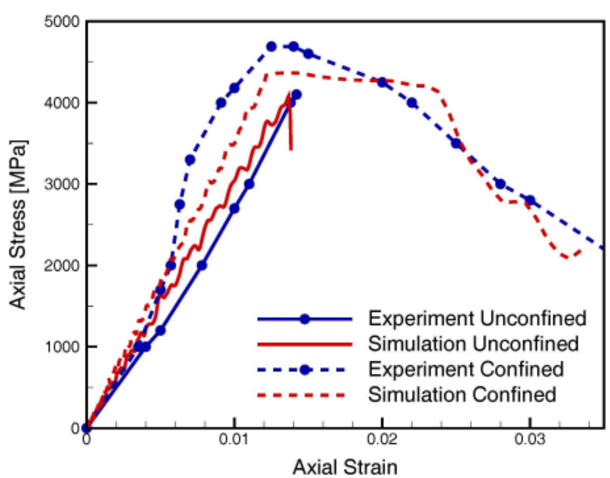




## Integrative Experiments

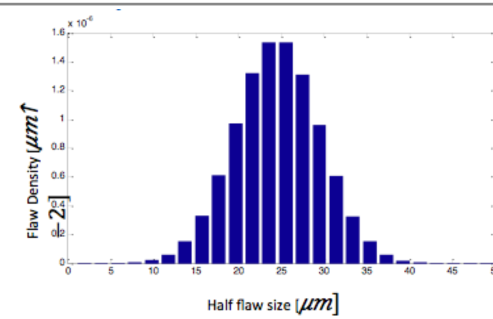
# Boron Carbide: Modeling and Scale-Bridging

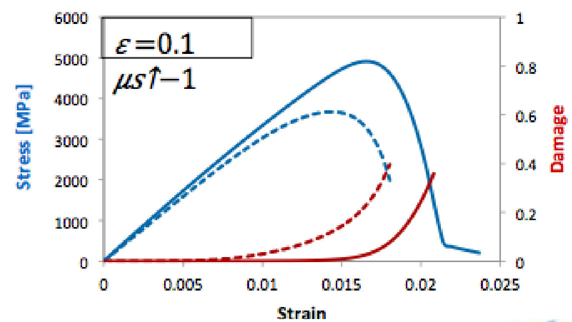
OTM Simulations of Massive Dynamic Failure

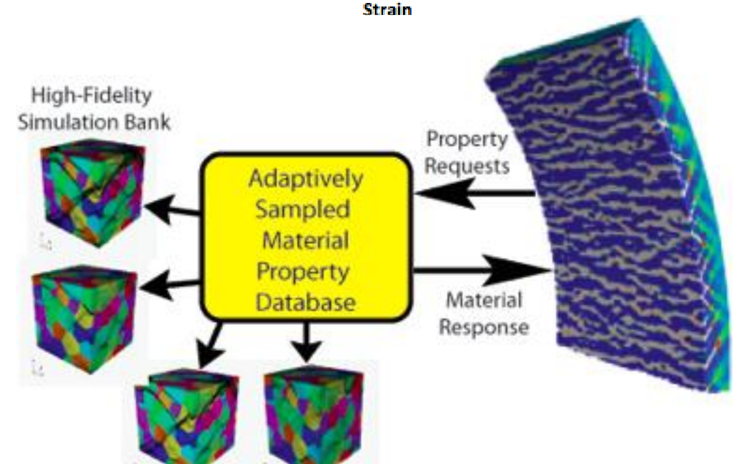


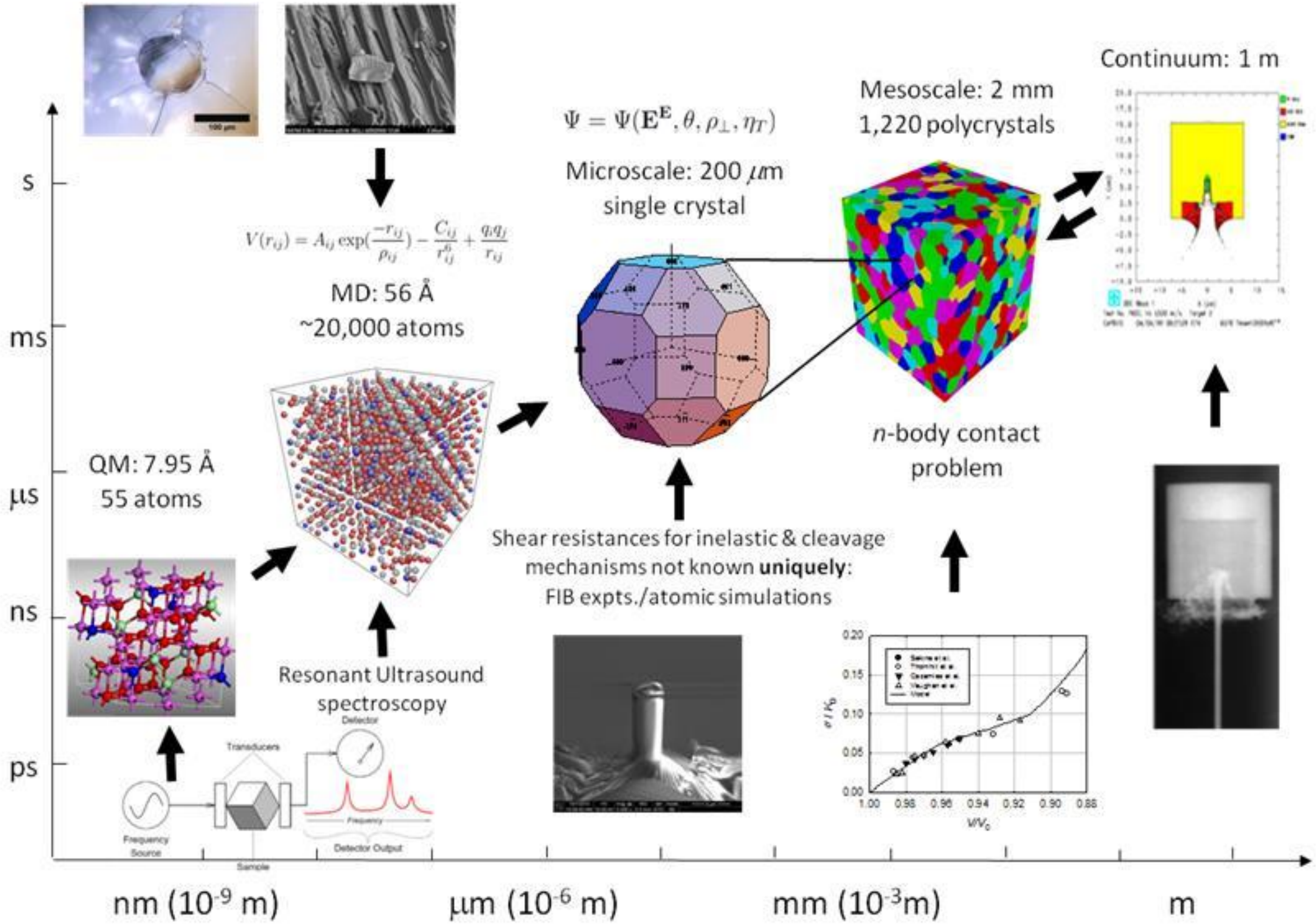

Failure of Unconfined and Confined Boron Carbide



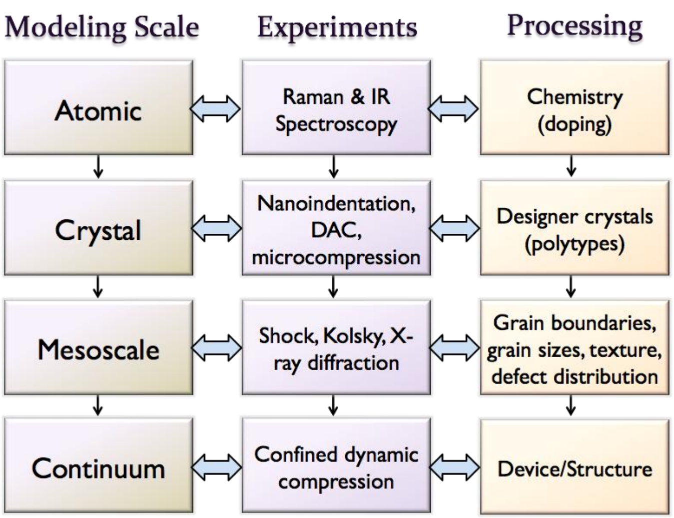



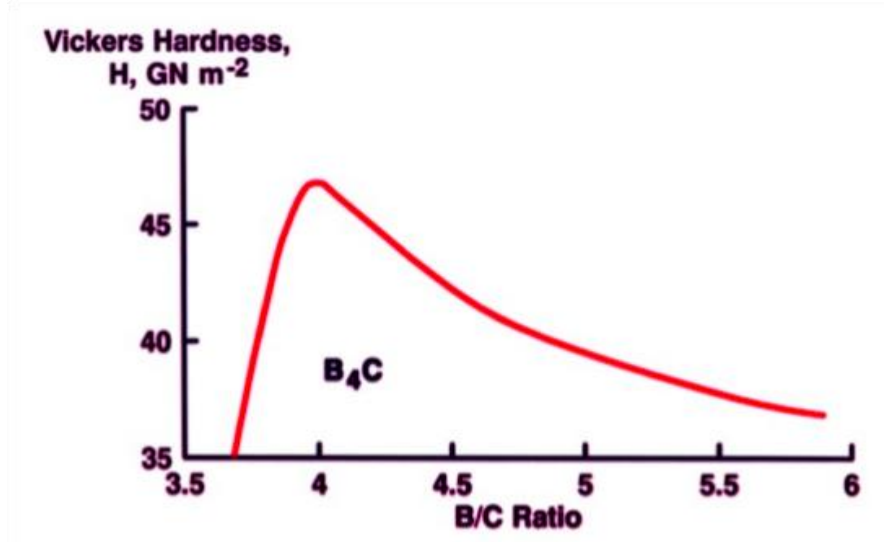



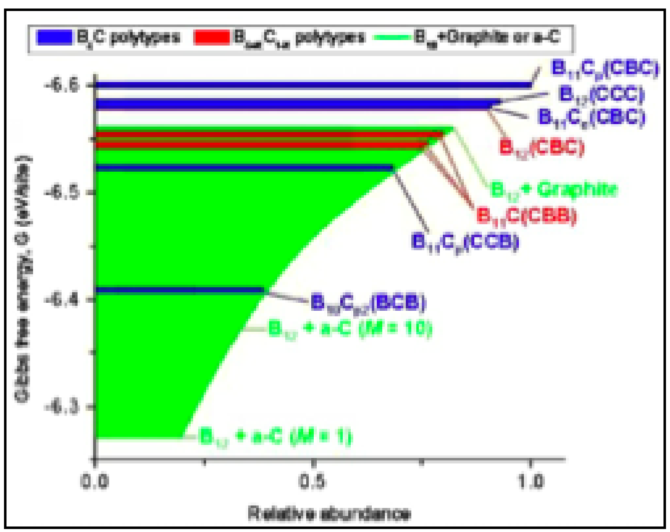
# Multiscale Modeling of Ceramics



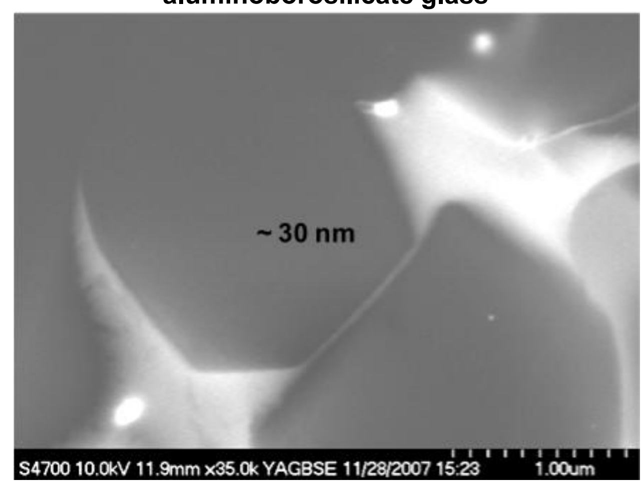
# Boron Carbide: Synthesis and Processing




Boron carbide 20 vol.% Y-doped aluminoborosilicate glass



# State of the Art for Polymers (PE, Epoxy)

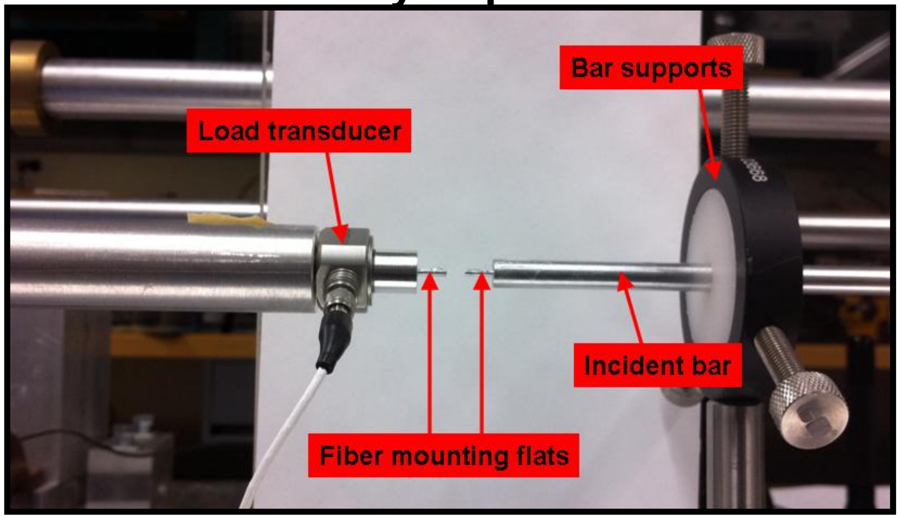
| Scale or Technical Core Element | Primary Mechanism | Advanced Exp. Tech. -1- | Modeling & Simulation -2- | Bridging Scales -3- | Material Char. & Prop. -4- | Synthesis & Processing -5- |
|---|---|---|---|---|---|---|
| **Atomistic/ Molecular -a-** | *Thermal motion, Chain conformation changes, Crystallinity, Bond rupture* | Flash DSC(Tg, Tm) In situ XRD, FTIR, In situ Electron Diffraction | All atom MD simulations | Coarse-grained potentials, models | Molecular conformation, Orientation, Molecular relaxation times, Molecular stiffness | Irradiative crosslinking of linear chains, Crystallization catalysts, Development of new catalysts for linear polymers |
| **Nano/Meso (Filament phase domains) -b-** | *Local defects motion (chain ends, kinks, entanglements), Chain orientation and stretching, Crystal/amorphous interphase* | High strain rate filament testing, In situ XRD, FTIR, Polarized Light Microscopy, High strain rate interface testing | MD simulations –united atom / coarse-grained; Constitutive models for domains, interphase | Coarse and fine-graining – hierarchical and simultaneous, time-temperature scaling , defect dynamics | High rate – properties, Crystal morphology, % crystallinity, Surface morphology and chemistry, Crystal orientation, Intermolecular shear strength | Surface modification, Draw ratio, Fiber diameter, Annealing steps, Molecular weight, End group termination |
| **Continuum (Filaments) -c-** | *Viscoelasticity Plasticity Strain hardening Fracture patterns Domain evolution* | High rate testing (SPHB, Shock), in situ WAXD | FEM, EOS, Homogenization | Coupled atomistic and continuum calculations of deformation and fracture | Viscoelastic, Viscoplastic Shock EOS | Cure kinetics, Process parameters (temperature, time, pressure) |



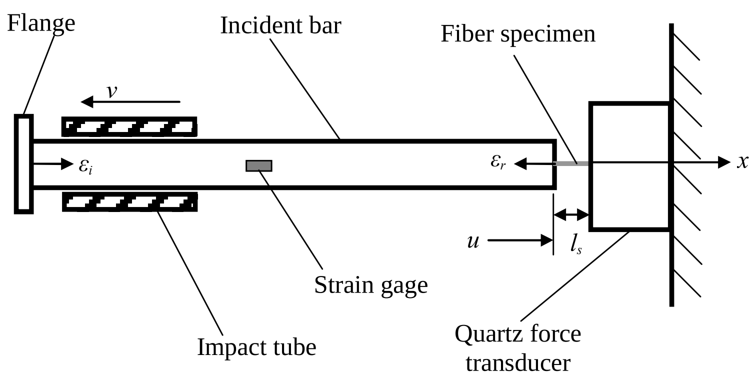
| Generally identified, understood or implemented | Sometimes identified, some understanding, some implementation | Weak identification understanding, or implementation | Poorly identified, poorly understood, or early implementations | Not identified, not understood or not implemented |
|---|---|---|---|---|

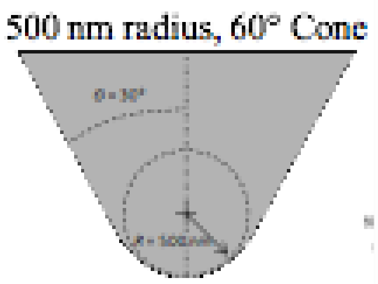
# UHMWPE: Experiments and Characterization

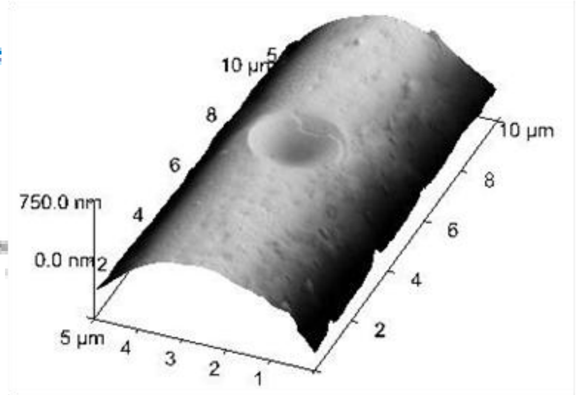
## Discovery Experiments

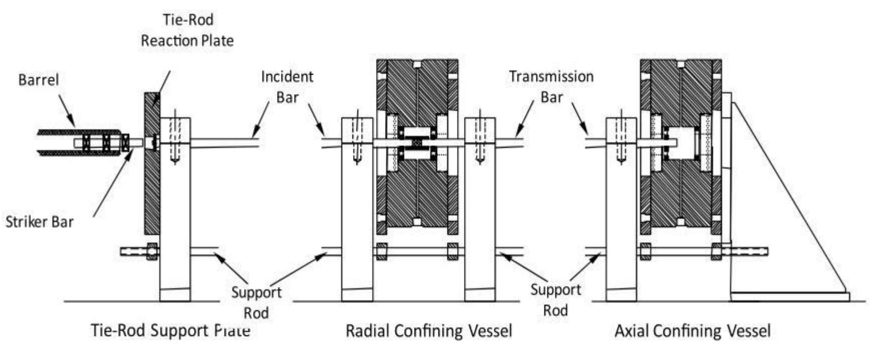



Unique High Loading-Rate Apparatus for Single-Fiber (~10 um diameter) Experiment



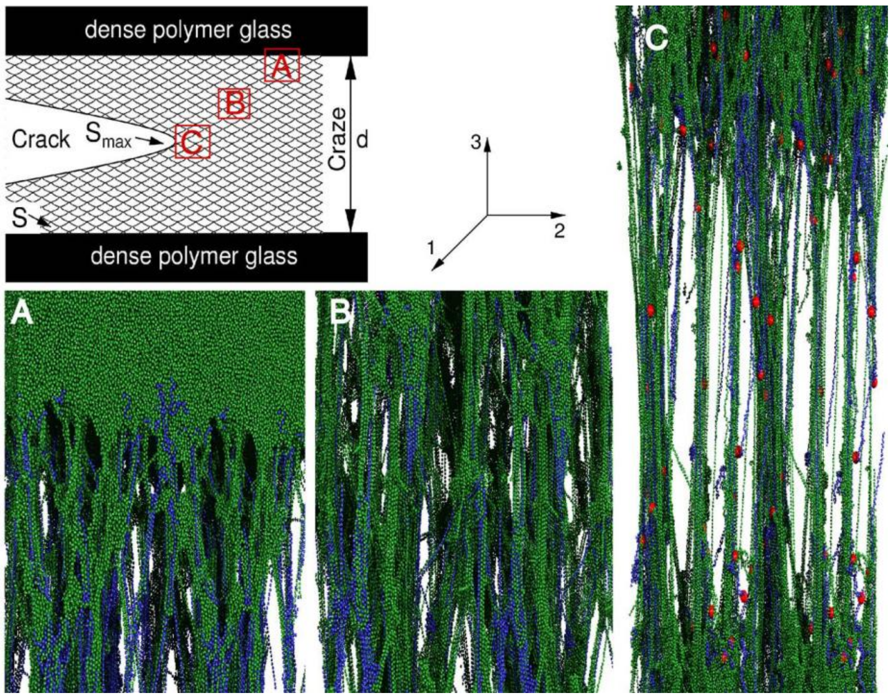




## Integrative Experiments

# UHMWPE: Modeling and Scale-Bridging



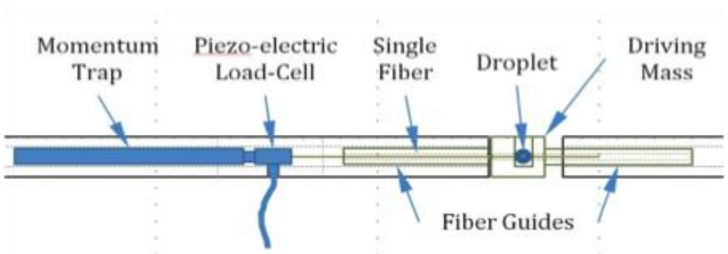

Crystalline and Amorphous Domains

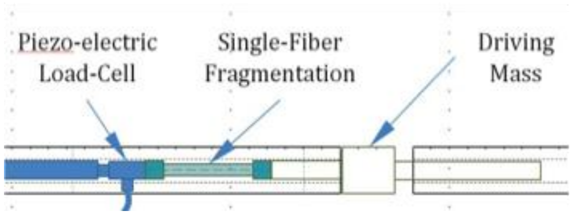
# State of the Art for Composites (S-glass-Epoxy)*

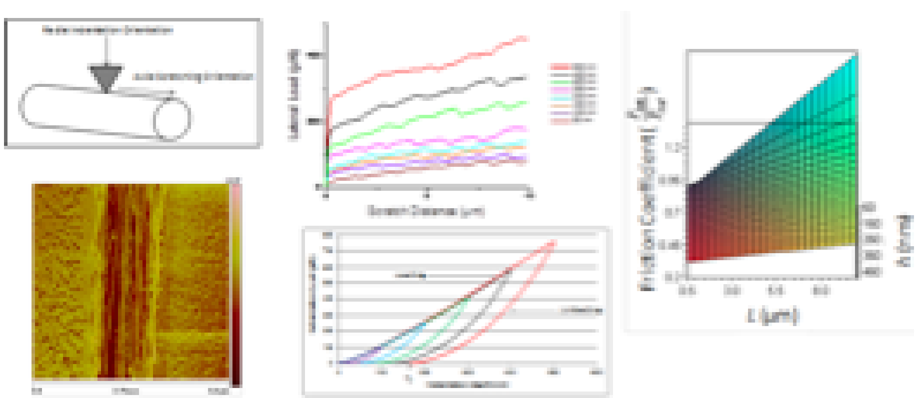
| Scale or Technical Core Element | Primary Mechanism | Advanced Exp. Techniques -1- | Modeling & Simulation -2- | Bridging Scales -3- | Material Characteristics -4- | Synthesis & Processing -5- |
|---|---|---|---|---|---|---|
| **Molecular (Network polymer) -a-** | *Network deformation Crosslink density Network connectivity Nanocavitation Relation to Tg* | High strain rate testing, In situ XRD, FTIR, Polarized Light Microscopy, High strain rate interface testing | MD simulations of networks to describe failure behavior of model networks | Development of constitutive relationships based on MD simulations | Distribution of crosslinks and mobility as a function of T relative to Tg, local network deformation - nanocavitation | Design of networks containing passive protovoids and thermally activated protovoids |
| **Nanoscale (Interphase) -b-** | Debonding , fiber pull-out, sliding friction, interphase failure | High rate interphase test methods (DILA, modified droplet, fragmentation etc.) | Peridynamic EMU, LS-Dyna, FEA, Cohesive zone | Nano- to micro-scale force potentials, Peridynamics, homogenization methods | Rate dependent interphase strength and energy dissipation | Interphase chemistry, fiber surface texture, resin wetting of textured fiber |
| **Microscale (Fiber/tow) -c-** | Fiber fracture (tension, compression), Fiber shear, Fiber crush, Statistical strength distributions | High rate filament/bulk testing, High speed photography, Fiber indentation | Peridynamics EMU, LS-Dyna, FEA | Peridynamics, homogenization methods (HCDM) | High rate nonlinear properties of filaments and composite tows, statistical strength distributions | Fiber sizing and surface treatments, filament count, yarn twist |
| **Mesoscale (Weave Architecture -d-** | Delamination, matrix cracking, micro buckling, friction, strain rate sensitivity, crack propagation, wave propagation and interaction | High rate testing (SPHB and Shock), Dynamic Yarn pullout, delamination (butterfly, wedge crack), High speed photography/DIC | FEA methods (LS-Dyna), Homogenization methods (HDCM), Peridynamic EMU, Analytical, Resin flow dynamics | Homogenization methods (HCDM), Coarse element, Non-linear micromechanics, RVE | Rate dependent non-linear stress-strain behavior, statistical property distributions, shock EOS | Fabric weave architecture control, fabric multi-scale permeability and resin flow |
| **Continuum -e-** | Matrix softening, delamination and friction, fiber tension and compression shear, fiber crush, compressibility | High rate testing (SPHB, Shock, Ballistic), Composite property measurement | Micro-mechanics, failure envelopes, continuum damage models; Analysis using FEM, SPH, EFG, Cohesive Zone, Analytical | Homogenization theory (HCDM), RVE, multi-scale, Wave propagations across length scales, hierarchical approaches | Rate dependent non-linear stress-strain behavior, shock EOS, statistical property distributions | 2D and 3D fiber architecture, multi-layered constructions, resin flow and permeability |

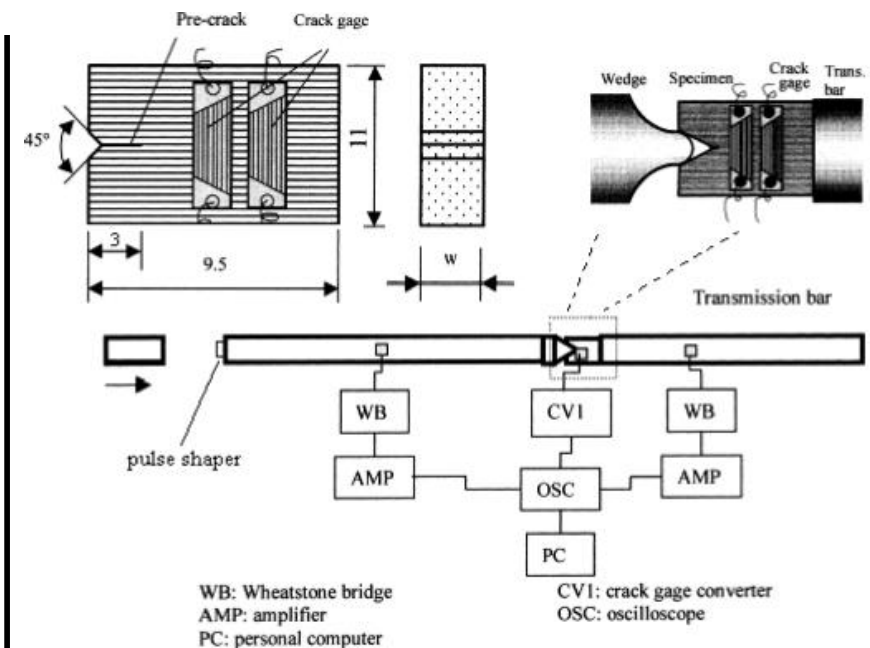
| | | | | |
|---|---|---|---|---|
| Generally identified, understood or implemented | Sometimes identified, some understanding, some implementation | Weak identification understanding, or implementation | Poorly identified, poorly understood, or early implementations | Not identified, not understood or not implemented |

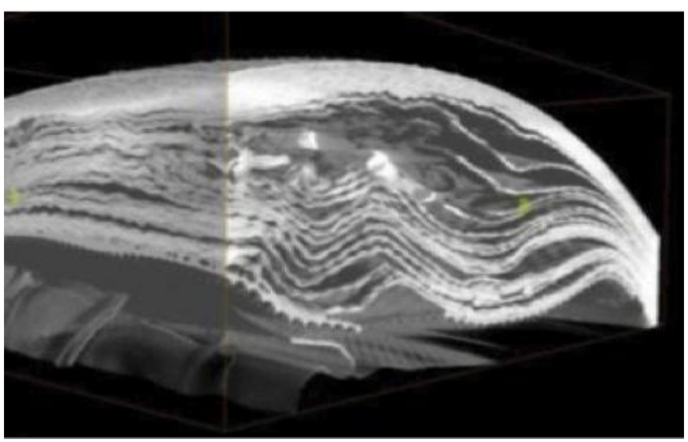
# S2-Glass Epoxy Composites: Experiments and Characterization



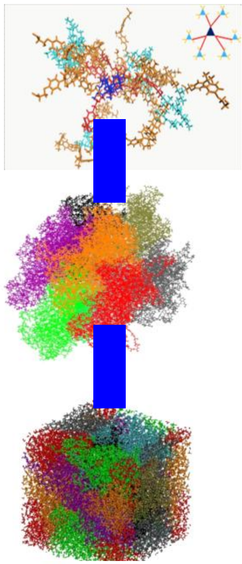



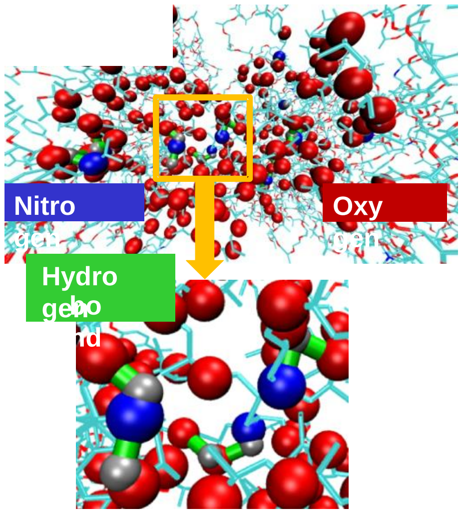





# S2-Glass Epoxy Composites: Modeling and Bridging the Scales

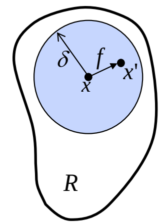


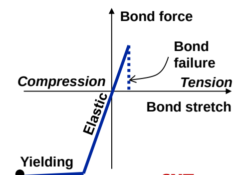


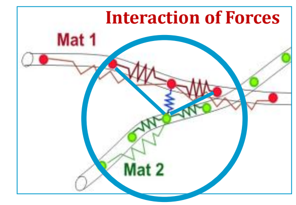

**PERIDYNAMIC INTEGRAL EQUATION OF MOTION**

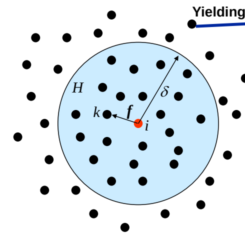
$$\rho\ddot{u}(x,t) = \int_R f(u'-u, x'-x)dV' + b(x,t)$$

- CONTINUUM VERSION OF MOLECULAR DYNAMICS
- ATOMISTIC-TO-CONTINUUM COUPLING
- MULTI-SCALE MODELING
- NANO-SCALE MODELING OF MATERIAL FAILURE

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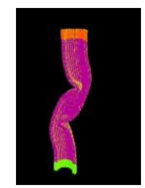
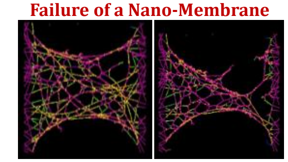


Failure of a Nano-Membrane

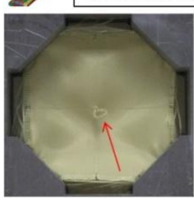


**Numerical Implementation**

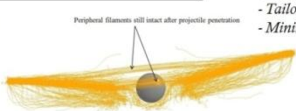
$$\rho\,\ddot{\mathbf{u}}_i^n = \sum_{k\in H} \mathbf{f}(\mathbf{u}_k^n - \mathbf{u}_i^n, \mathbf{x}_k - \mathbf{x}_i)\Delta V_i + \mathbf{b}(\mathbf{x}_i, t)$$

**Filament-Filament Interactions**

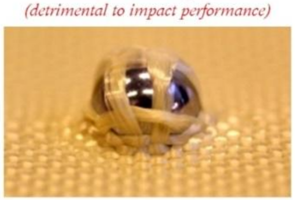
- *Engage all filaments, promote load sharing*
- *Tailor inter-filament, inter-yarn frictional interactions*
- *Minimize fabric windowing*

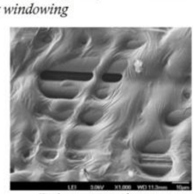


Fabric penetration via windowing and principal yarn pullout – no yarn failure



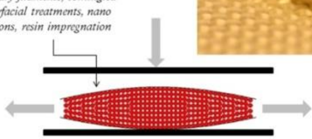

Fabric Windowing Effect
*(detrimental to impact performance)*



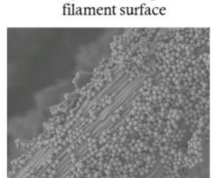


Polymer coating on filament surface

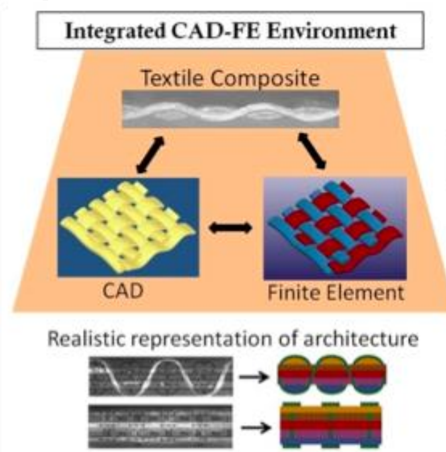
**Effect on Filament Spreading:**
*Friction, twist, dry filaments, comingled filaments, interfacial treatments, nano particle inclusions, resin impregnation*

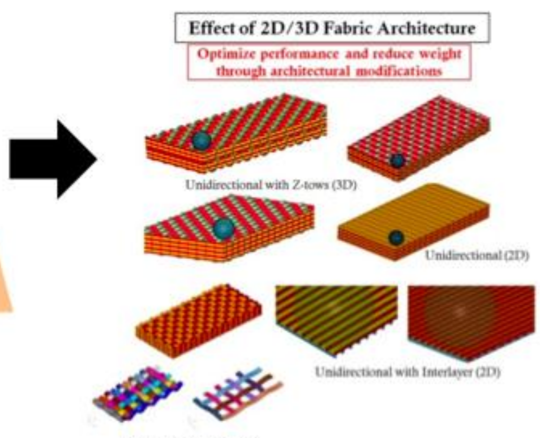


Filament redistribution under transverse load

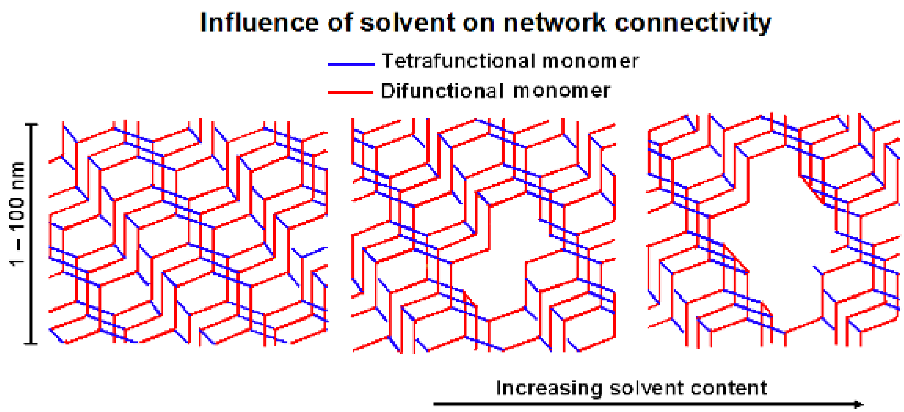


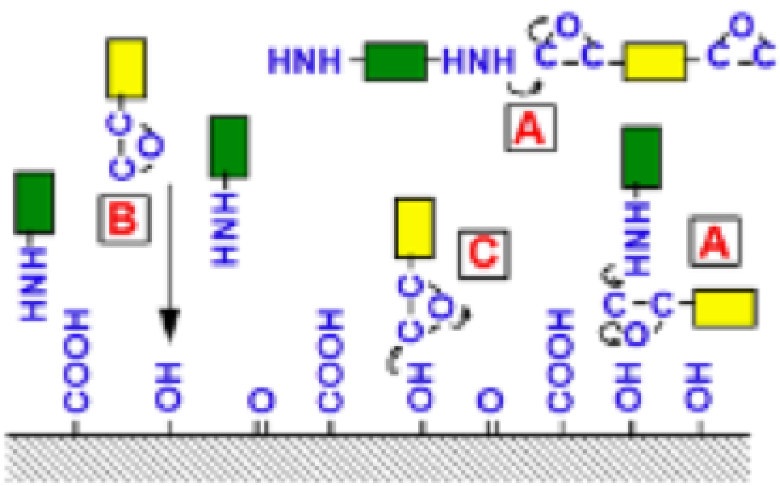
Nano particles on filament surface:
*Indentation and gouging*

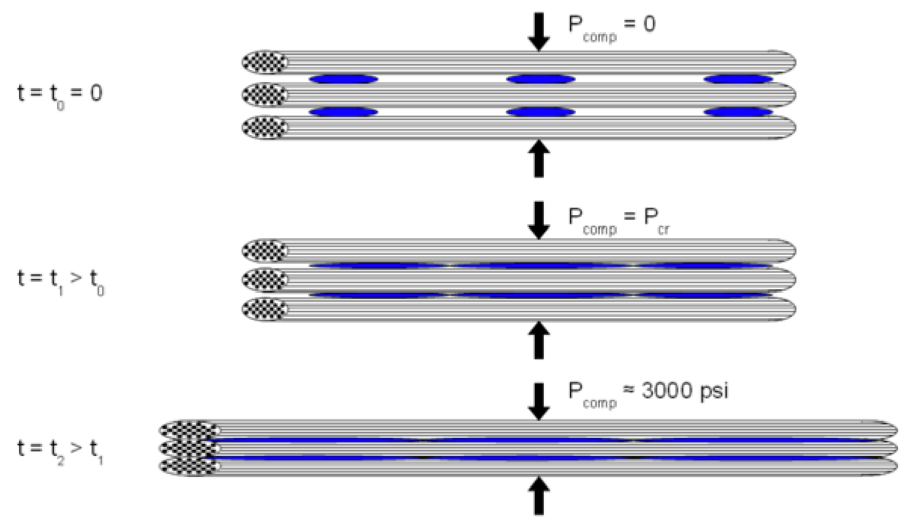


# S2 Glass Epoxy Composites: Processing and Synthesis



# MEDE Collaboration Challenges

- Challenge: how to translate materials needs for armor applications to basic scientific research in an open scholarly setting?
  - Canonical model is the key to this connection
- Challenge: how to get this large, geographically dispersed group to work together effectively?
  - Develop a structure that connects research groups along multiple dimensions of individual interests (by material class, by common research tools)
  - Develop an infrastructure that supports collaboration (data sharing, collaborative space, facilitate visits)

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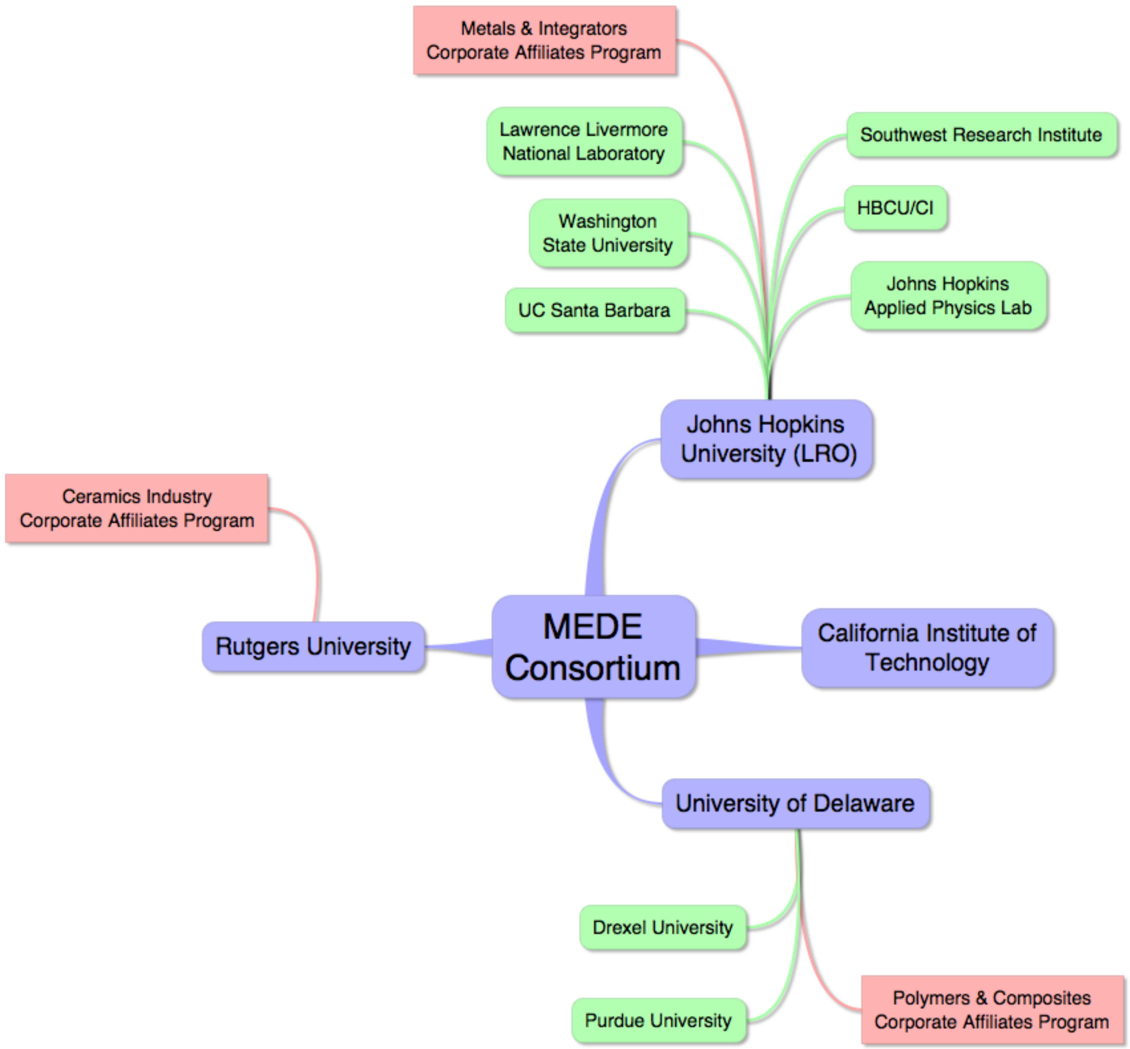
# Size/scope of MEDE CRA

ARL




- 40+ faculty/senior researchers
- 40+ graduate students/posdocs
- 40+ ARL scientists
- Many corporate partners, undergraduates, administrative staff
- ~150 active participants
- Collaboration is key

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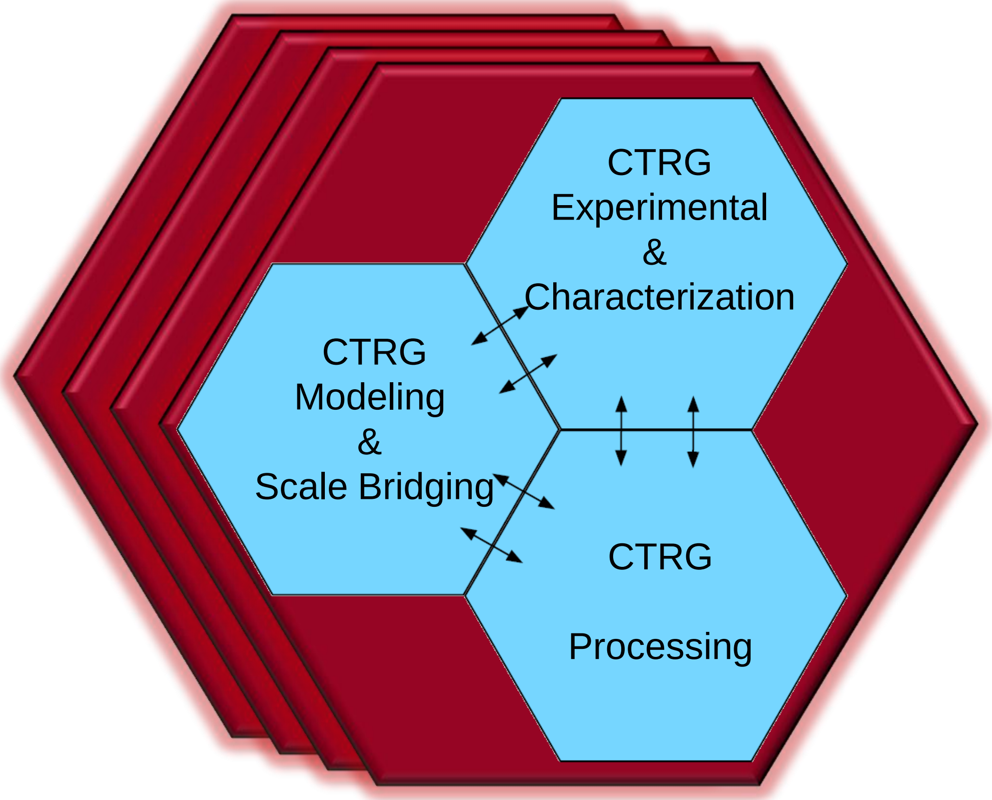
# Collaboration Mechanics

ARL

- **4 Collaborative Materials Research Groups (CMRG – red hexagons)**
- **3 cross-cutting themes that are uniform across CMRGs**
- **3 themes x 4 CMRG = 12 CTRG's**
- **CTRG: focal points for interaction between Consortium and ARL researchers with similar interests**
- **Regular meetings are structured around both CMRG and cross-cutting CTRG themes**
- **Software/tools coordination committee**



# MEDE Collaborative Plans

- **Regular meetings (details next slide)**
- **Regular visits between ARL and Consortium, in both directions**
- **Development of computational infrastructure for sharing data**
- **Establish collaborative space, both at Consortium and at ARL**
- **Educational efforts**
- **MEDE Corporate Partnership Program - currently ~90 members**
- **Contribute to the science of collaboration:**

***HEMI as a testbed for JHU Systems Institute to study information flow in collaborative networks and help to identify best practices***

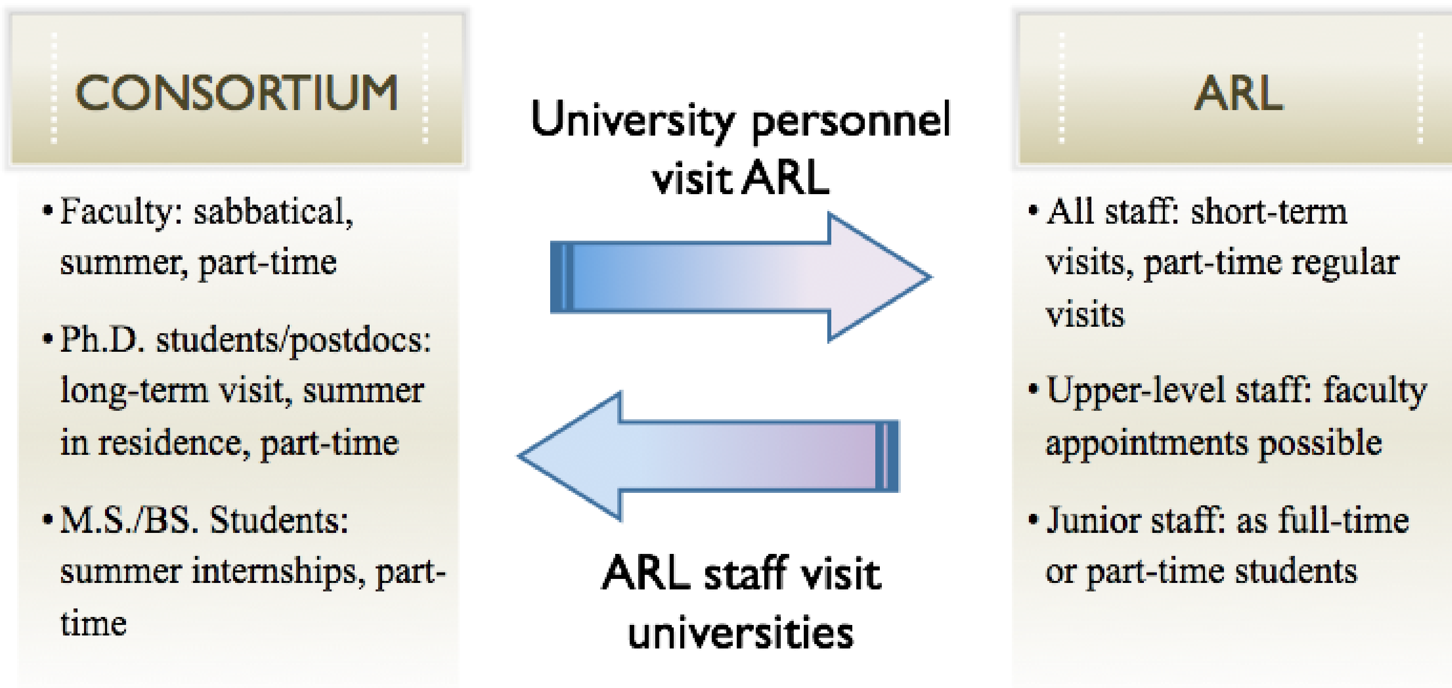
# MEDE Collaborative Plans

- Regular meetings, with the following rough quarterly schedule:
  - *Winter*: CTRGs meet in context of CMRG, time/location set by individual CMRG
  - *Spring*: MEDE Conference, open to broad scientific community (CTRG meetings held here, as well as Codes/Tools Coordination Committee)
  - *Summer*: CTRGs meet in context of cross-cutting themes, time/location set by individual cross-cutting themes
  - *Fall*: MEDE Workshop, meeting of entire MEDE community (CTRG meetings held here, as well as Codes/Tools Coordination Committee)

# MEDE Collaborative Plans



- Regular visits between ARL and Consortium, in both directions



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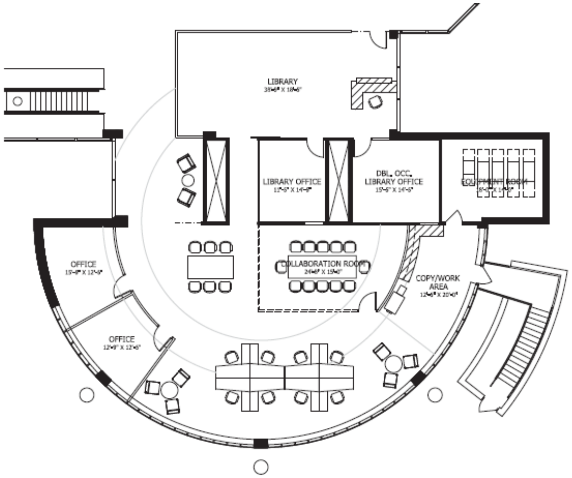
# MEDE Collaborative Plans

ARL

•**Establish collaborative space, both at Consortium and at ARL**

Future home of MEDE at JHU, Malone Hall to be completed Spring 2014




ARL is pursuing new collaborative computational facilities

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# Take-Aways from MEDE

ARL

We have established a great team

Collaboration-Collaboration-Collaboration

NOT a collection of individual projects

The goal is not just better Mg, B4C, UHMWPE & Composites, but the ability to design future materials for future defeat mechanisms for future armors for future threats

Cross-cutting themes will form the foundation for future success for the ARL Enterprise

**FUTURE PAYOFF** Vehicle and Soldier Protection - 1/3 savings in weight