Molecular Design of Composite Constituents

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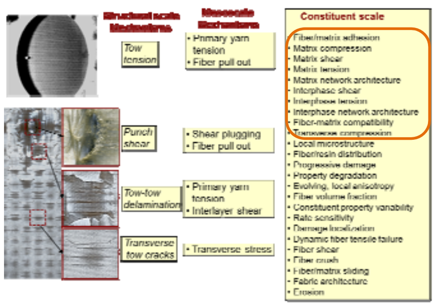
Enterprise for Multi-scale Research of Materials

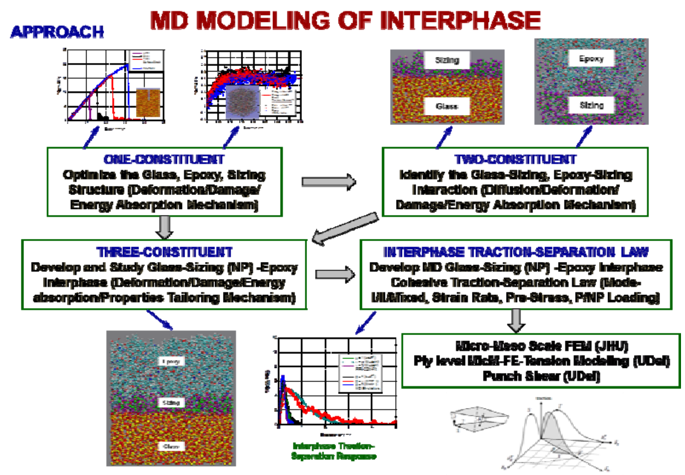
How We Fit

Materials-by-Design Process

Mechanism-based Approach



Technical Approach



Key Accomplishments

- *New Energy Absorbing Epoxies*
- *MD Prediction of Interphase Traction laws for Bridging Length Scales*
- *Prediction of Glass Fiber HSR Properties*
- *Materials by Design Framework Established*

Future Directions

- *Advance MD models for three constituents*
- *Optimize interphase properties*
- *Validate predictions through canonical testing*

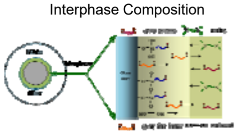
Impact

- *New energy absorbing mechanisms*
- *New light weight protection materials*
- *Validated multi-scale models for Design of Next Generation Soldier Systems*

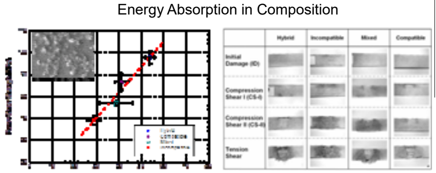
Goals and Motivation

- **Model and control high strain rate mixed-mode traction-separation laws for glass fiber/epoxy interphases**
- **Develop a 'Materials-By-Design' methodology to bridge length scales from Molecular Dynamics (MD) into finite element (FE) (potential based cohesive modeling)**
- **Advance basic understanding of:**
  - **load transfer within interphase under HSR**
  - **role of sizing and resin chemistry**
  - **energy absorbing mechanisms from nanometer to micron length scales**

Interphase Composition

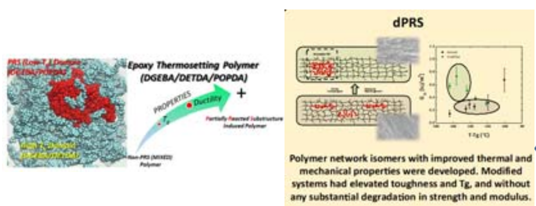


Interphase Design Improves Strength and Energy Absorption in Composition



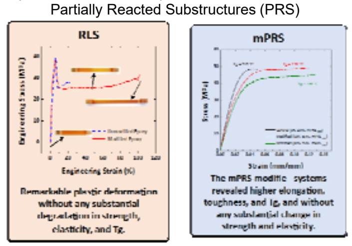
Major Results

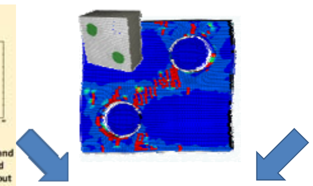
MD Epoxy: New Energy Absorption Mechanisms



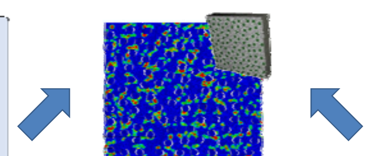
Synthesis of New Epoxy Networks and Interphases Partially Reacted Substructures (PRS)

MD simulations of coarse-grained PRS systems

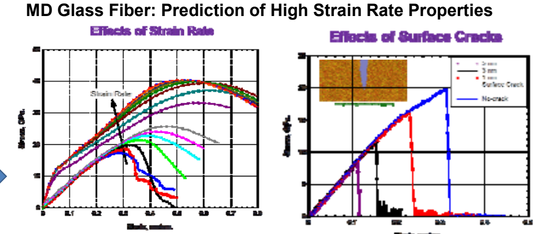




Inputs to RVE Scale Micromechanical Damage Models

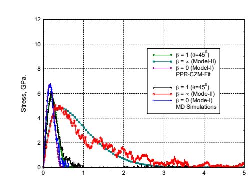


MD Glass Fiber: Prediction of High Strain Rate Properties



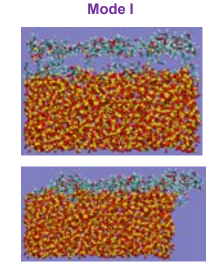
MD Interphase Design: Prediction of Traction Laws for Bridging Length Scales

Mixed Mode Potential Based Cohesive Zone Model



Code implementation include load/unloading capability

Mode I



Mode II

CMEDE — CENTER FOR MATERIALS IN EXTREME DYNAMIC ENVIRONMENTS

University of Delaware — Drexel University