# Multi-Scale Modeling of Fiber-Matrix Interphase

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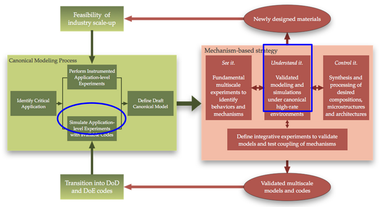
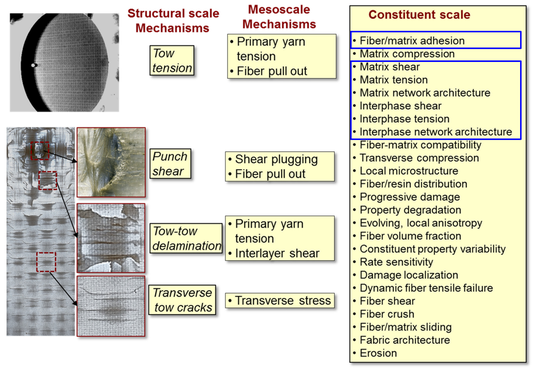
Enterprise for Multi-scale Research of Materials

## How We Fit

### Materials-by-Design Process

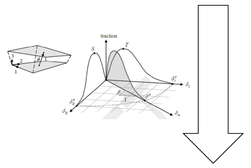



### Mechanism-based Approach

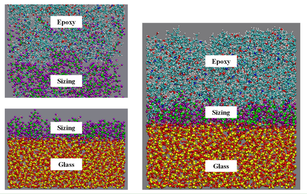



## Technical Approach

**Molecular Modeling of Single-Constituent Systems (Glass, Sizing & Epoxy) (Study Energy Absorption & Damage Mechanism)**




**Molecular Modeling of Two-Constituent Systems (Glass-Sizing, Epoxy-Sizing) (Study Diffusion & Degree of Adhesion)**



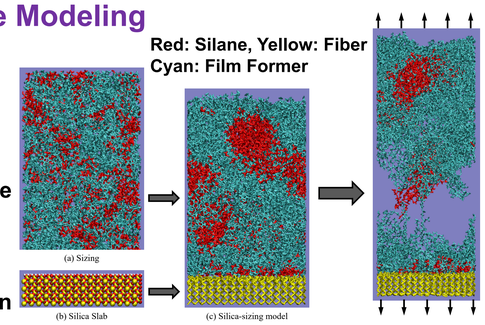

**Molecular Modeling of Three-Constituent Glass-Sizing-Epoxy Interphase (Deformation/Damage/Energy absorption/Properties Tailoring Mechanism)**

**Develop Interphase Cohesive Traction-Separation Law (Mode-I/II/Mixed, Strain Rate, Pre-Stress, Proportional/Non-Proportional Loading)**

## Major Results/Key Accomplishments

### Silica-Sizing Interphase Modeling

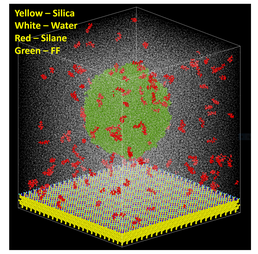
- ✓ Silane molecules agglomerate and make macromolecules creating heterogeneous structure
- ✓ Some silane molecules are attracted to the silica surface (0.5 – 0.7 GPS/nm$^2$)
- ✓ Damage initiates and propagates in the uncross-linked film former rich region




## Path Forward

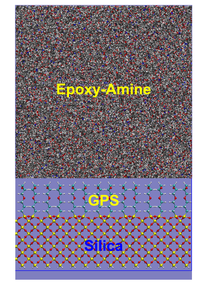
### Aqueous Sizing Modeling (Collaboration with Drexel)

- ✓ Identify sizing formation mechanism and its morphology
- ✓ Identify effects of pH and surfactant
- ✓ Understand the distribution of silane, shape and wettability of the FF particle after water evaporation



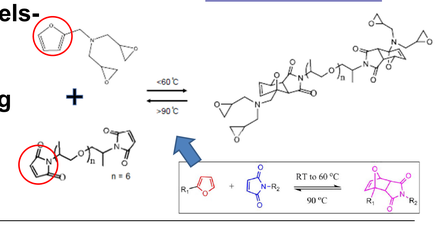

### Silica-GPS-Epoxy Interphase Modeling

- ✓ Identify damage mechanism and damage prone regions under mech. deformation
- ✓ Develop mixed-mode traction law (equivalent to zero thickness cohesive zone) by inserting crack in the damage prone region



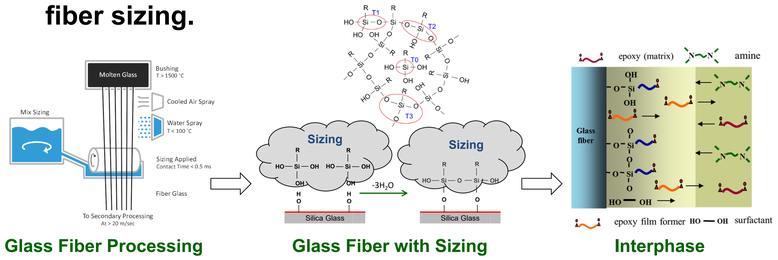

### DAS Modified Epoxy Modeling

- ✓ Reactive MD simulations of Diels-Alder Substructure (DAS) modified epoxy system to understand properties tailoring mechanism
- ✓ Conduct model validation experiment (Drexel)




## Key Goals

- Interphase is a distinct region between fiber and matrix which develops during processing through diffusion and reaction between the matrix and the fiber sizing.

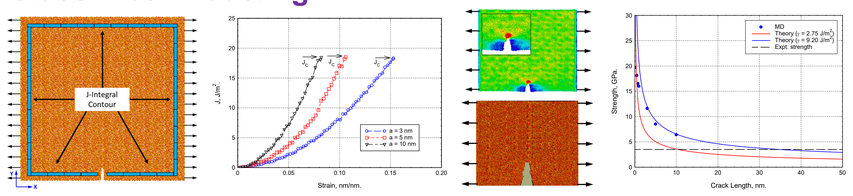



Glass Fiber Processing | Glass Fiber with Sizing | Interphase

- Establish a molecular dynamics based "Materials-by-Design" framework for composite interphase
  - ✓ Identify the interphase formation mechanism and its morphology at the atomistic level
  - ✓ Identify the interphase deformation and energy absorption mechanism
  - ✓ Develop mixed-mode traction law

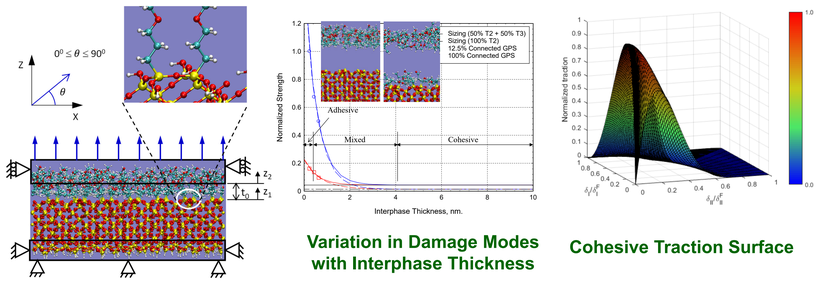
## Major Results/Key Accomplishments

### Glass Fiber Modeling




- ✓ Nanometer size surface cracks significantly reduce fiber strength
- ✓ Fracture toughness is determined through atomistic J-integral

### Silica-Silane Interphase Modeling




Variation in Damage Modes with Interphase Thickness | Cohesive Traction Surface

- ✓ Interphase strength increases with decrease in interphase thickness
- ✓ Strength improves significantly with increase in GPS bond density

## Transitions/Impact

- ✓ MD based materials-by-design framework will guide ARL/CMRG experimentalists to design optimum interphase structure
- ✓ MD based interphase mixed-mode traction law will be used in composites micro-mechanics damage modeling

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