How We Fit

Materials-by-Design Process

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)

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.

- 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

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 GPa/m²)
- Damage initiates and propagates in the uncross-linked film former rich region

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)

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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