Multi-Scale Modeling of Fiber-Matrix Interphase

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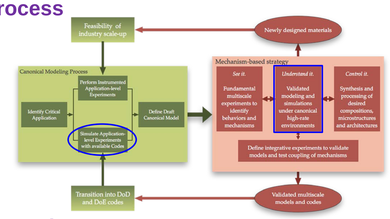
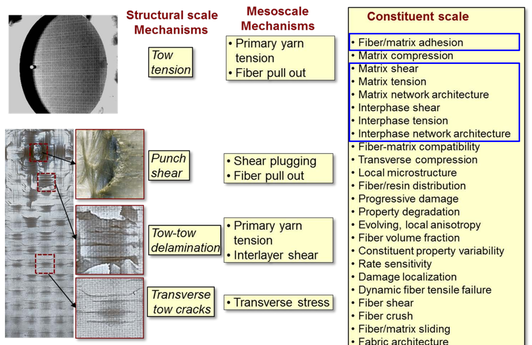
How We Fit

Materials-by-Design Process



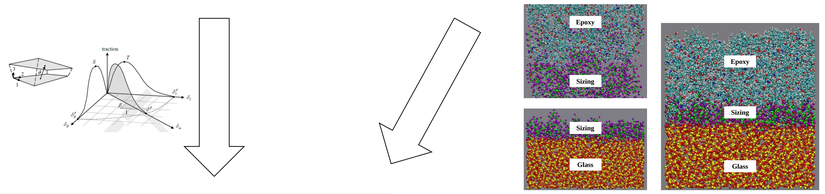
Mechanism-based Approach



Technical Approach

Molecular Modeling of Single-Constituent Systems (Glass, Sizing & Epoxy) (Deformation/Damage Mechanism)

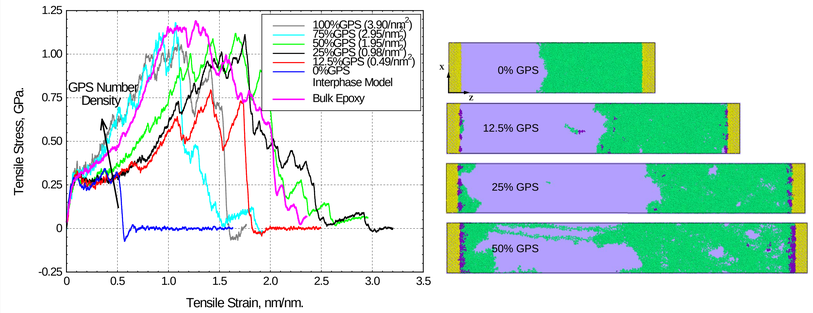
Molecular Modeling of Two-Constituent Systems (Glass-Sizing, Epoxy-Sizing) (Glass surface adhesion/inter-diffusion)



Molecular Modeling of Three-Constituent System Glass-Sizing-Epoxy Interphase (Formation, Deformation/Damage/Energy Absorption Mechanisms & System Optimization)

Develop MD Based Mixed-Mode Traction-Separation Law Surfaces (Strain Rate/Hydrostatic Pressure Effects)

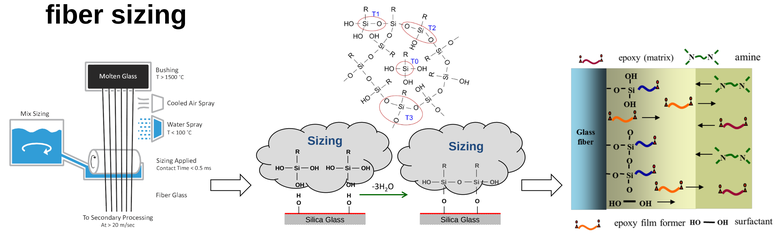
Major Results/Key Accomplishments



- ✓ **Overall, composite strength improves with increase in the silane (GPS) concentration**
- ✓ **At 0% GPS, failure is adhesive at fiber surface (Non-bonded interaction only)**
- ✓ **As GPS number density increase, cohesive failure occurs in the bulk epoxy**
- ✓ **At 50-75% GPS concentration, composite strength and energy reach bulk epoxy properties and failure modes transition to cohesive failure in epoxy**
- ✓ **MD prediction is consistent with the micro-mechanics based R-value analysis (Ganesh et al., JCM 2018)**
- ✓ **Development of mixed-mode TL is in progress**

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**



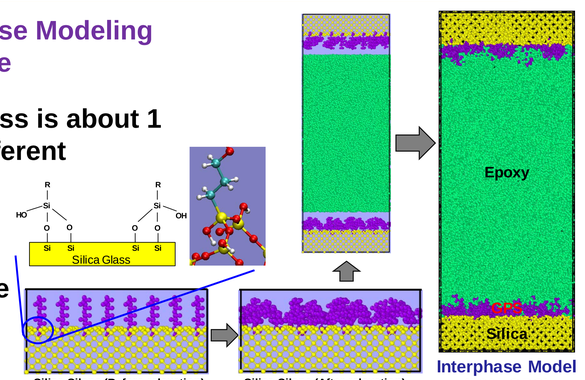
Glass Fiber Processing | **Glass Fiber with Sizing** | **Interphase**

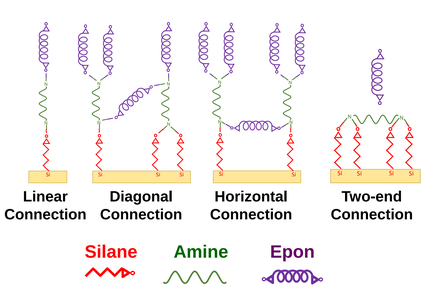
- ✓ **Establish a molecular dynamics based "Materials-by-Design" framework for composite interphase**
- ✓ **Bridge length scales using MD based mixed-mode cohesive traction law surfaces**
- ✓ **Design new composite interphases to improve composite performance based on CMRG integrative models and objective functions**

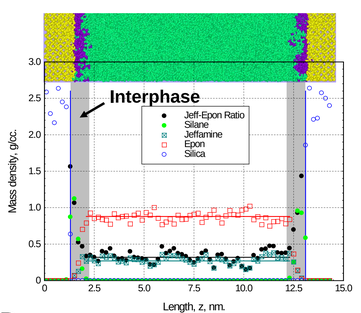
Major Results/Key Accomplishments

Fiber-Epoxy Interphase Modeling with Monolayer Silane

- ✓ **Interphase thickness is about 1 nm consists of different connectivity patterns**
- ✓ **Diagonal type pattern is favorable to increase strength and energy absorption**







Path Forward

- ✓ **MD based interphase design for the CMRG uniaxial tension and punch shear integrative models**
- ✓ **Study the effects of fiber breakage on energy dissipation - interphase de-bonding and matrix cracking**

Transitions to ARL, within CMRG and to other CMRGs

- ✓ **Developed MD protocol will be transitioned to ARL**
- ✓ **MD based interphase mixed-mode traction law will be used in composites micro-mechanics damage modeling**

Contribution to MEDE Legacy

- ✓ **MD based materials-by-design framework will guide ARL/CMRG experimentalists to design optimum interphase structure**

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