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**How We Fit**

Materials-by-Design Process

- Establish a molecular dynamics based “Materials-by-Design” framework for composite interphase
- Identify the interphase (fiber-sizing-epoxy system) deformation and energy absorption mechanism
- Predict traction law – Mode I, II & Mixed Mode
- Predict strain rate, pre-stress effects on TL

**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 (fiber-sizing-epoxy system) deformation and energy absorption mechanism
- Predict traction law – Mode I, II & Mixed Mode
- Predict strain rate, pre-stress effects on TL

**Major Results/Key Accomplishments**

- Epoxy with low molecular weight cross-linker has better thermomechanical properties
- ReaxFF can capture the damage through bond breakage

<table>
<thead>
<tr>
<th>System</th>
<th>Modulus (GPa)</th>
<th>Yield Strength (GPa)</th>
<th>Tg (K)</th>
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<tr>
<td>Epon828-Jeff130</td>
<td>5.16</td>
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<td>Epon828-Jeff600</td>
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</tbody>
</table>

- Sizing morphology affects its properties
- Though presence of more T3 molecules gives better mechanical properties, these structures should have less adhesion with fiber surface

**Future Directions in 2017**

- Study two- and three-constituent systems interaction
- Predict traction law for these systems at high strain rate
- Conduct model validating experiment for interphase and its constituent systems at high strain rates

- Silane based interphase should be created in between two quartz substrates
- Samples should be tested at various angles for mixed failure modes at high strain rates using SHB