Multi-Scale Modeling of Fiber-Matrix Interphase

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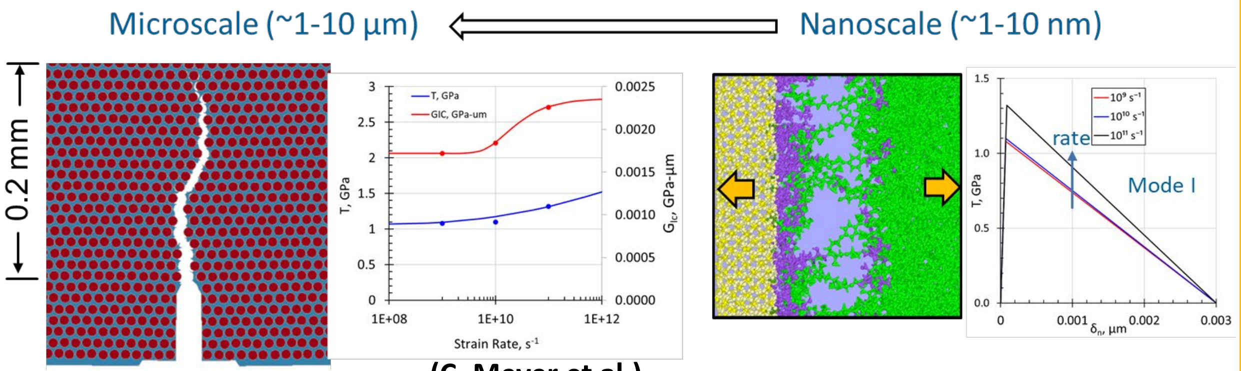
Key Goals and Technical Approach

- ✓ Establish 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 integrative models and objective functions

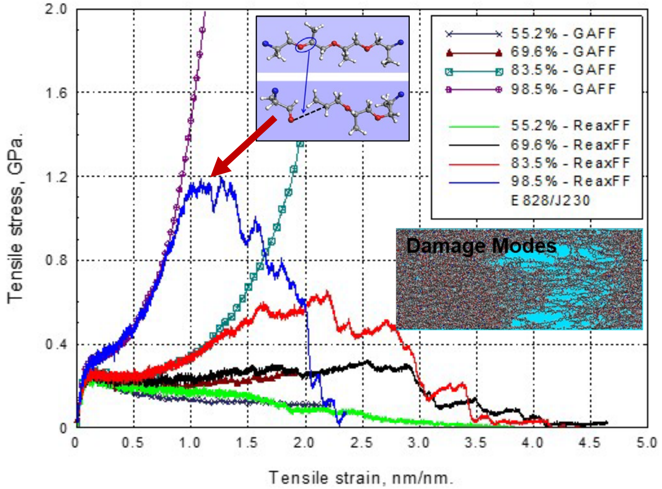


(C. Meyer et al.)

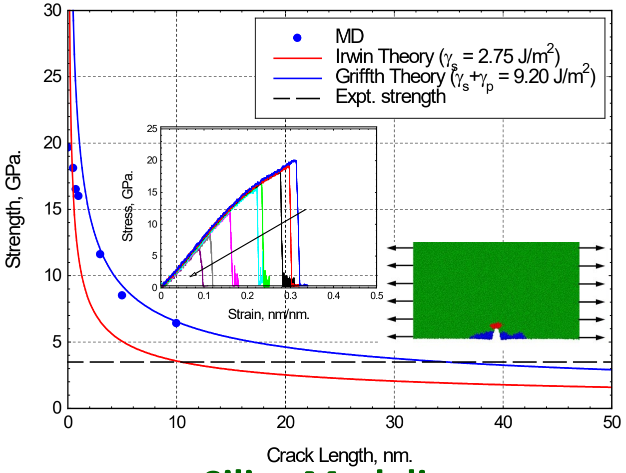
- ✓ Systematically Study
  - Single Constituents: Glass, Epoxy & Sizing
  - Two Constituents: Glass-Sizing Interaction
  - Three Constituents: Fiber-Matrix Interphase with Silane

Single Constituent Modeling

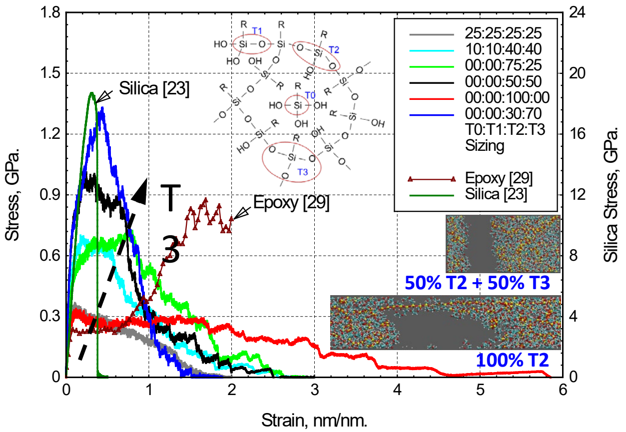
- ✓ Single constituent glass, epoxy and sizing are studied with reactive force field ReaxFF to establish the structure-properties relationship
- ✓ Understand the deformation, damage and properties tailoring mechanism at the atomic length scale
- ✓ Develop strain-rate dependent constitutive model



Epoxy Modeling



Silica Modeling



Sizing Modeling

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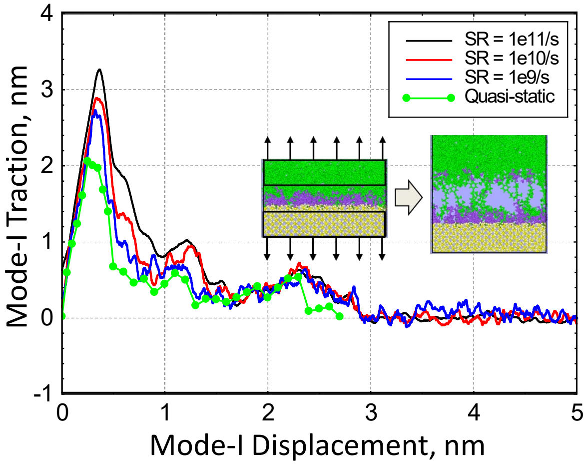
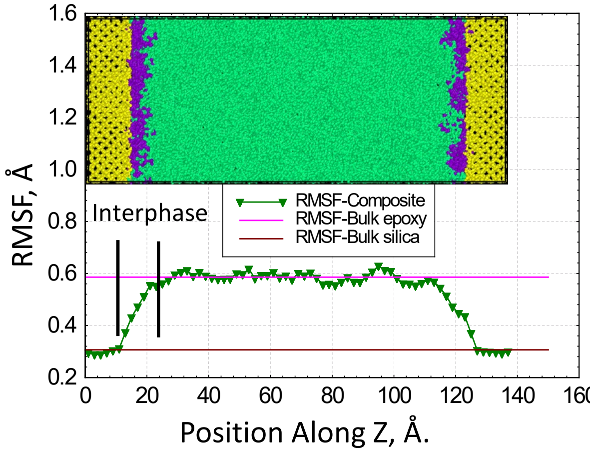
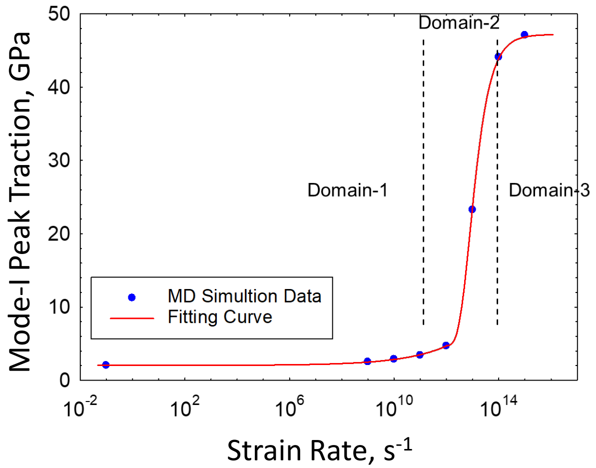
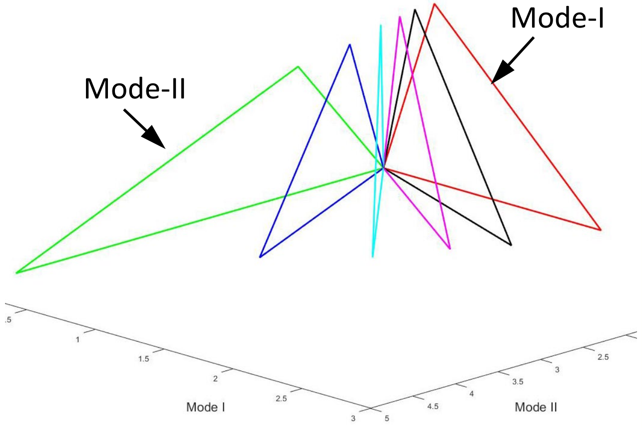
Rate-Dependent Interphase Traction Laws

- ✓ Develop strain-rate dependent mixed-mode traction laws as a function of interphase structure
- ✓ Introduce stress-relaxation approach to predict quasi-static response









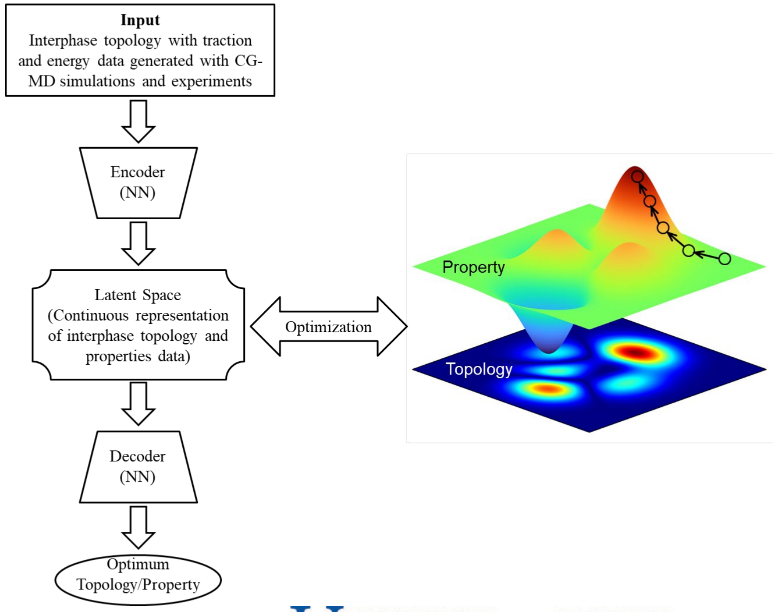
- ✓ Investigate the effects of fiber surface roughness and transverse pressure

Transitions (materials, codes/tools, legacy publications)

- ✓ MD framework for fiber-matrix interphase modeling
- ✓ Atomistic models, codes and other data will be uploaded to Craedl and shared with ARL
- ✓ Materials-By-Design mixed-mode, strain rate and pressure dependent traction laws for bridging length scales in composite modeling
- ✓ Twenty one journal and conference papers are published from this MD modeling projects over last few years, which are uploaded to CRAEDL

Path Forward

Develop physics informed machine learning (PIML) framework considering wide range of resin and coupling agent chemistry, variability in interphase topology in case of multi-layer silane, and pressure/temp/strain rate effects



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