Multi-Scale Modeling of Fiber-Matrix Interphase

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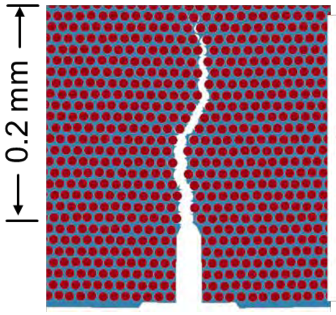
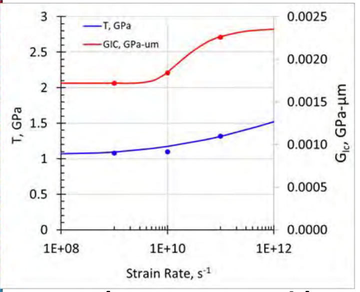
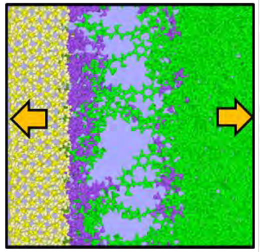
Key Goals and Technical Approach

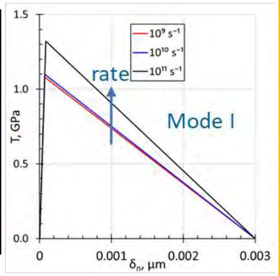
- ✓ Establish molecular dynamics-based “Materials-by-Design” framework for composite interphase
- ✓ Bridge length scales using MD-based mixed-mode cohesive traction law surfaces
- ✓ Design new composite interphases to improve composite performance based on integrative models and objective functions

Microscale (~1-10 μm) ⟵ Nanoscale (~1-10 nm)







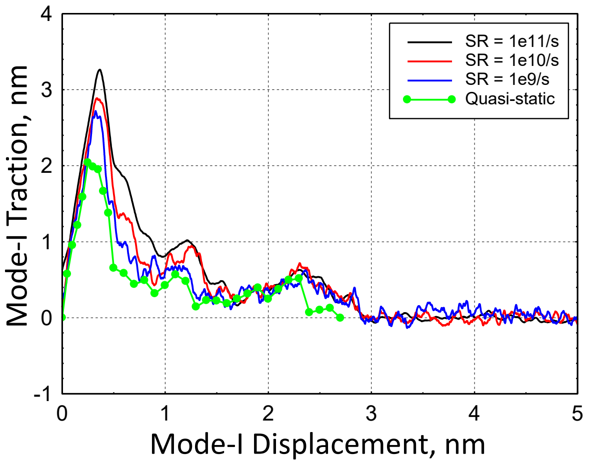


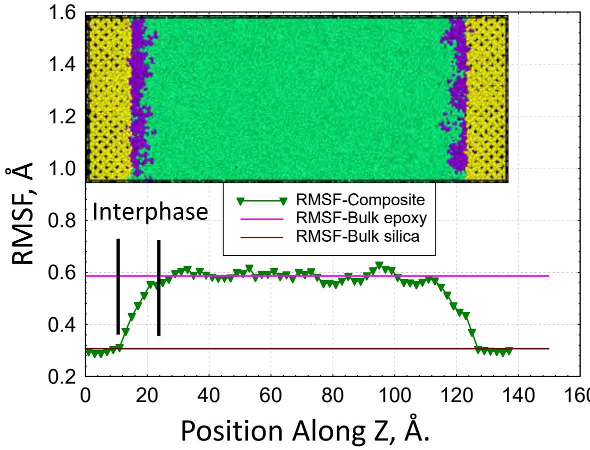
(C. Meyer et al.)

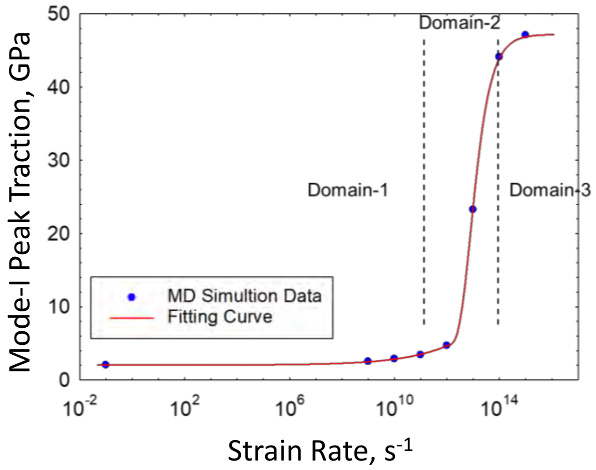
- ✓ Systematically Study
  - Single Constituents: Glass, Epoxy & Sizing
  - Two Constituents: Glass-Sizing Interaction
  - Three Constituents: Fiber-Matrix Interphase with Silane

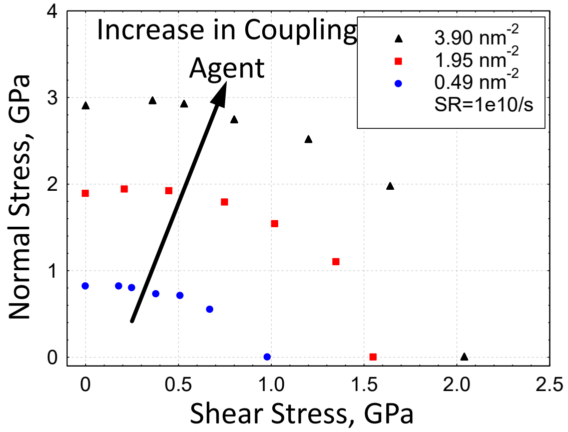
Rate-Dependent Interphase Traction Laws

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









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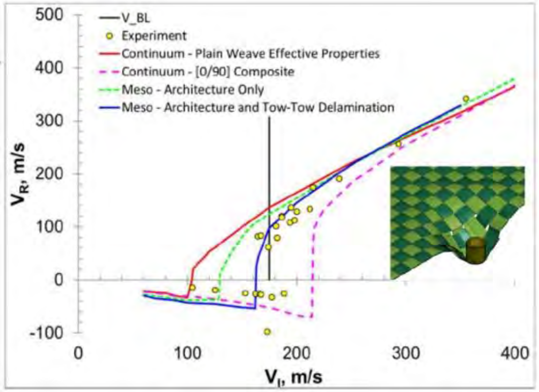
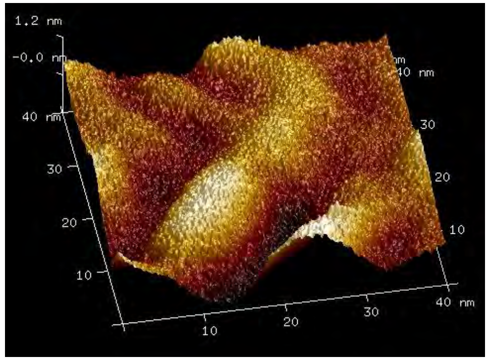
Transverse Pressure and Surface Roughness Effects

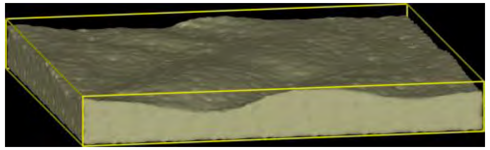
- ✓ Two sources develop radial compressive stress in composites - residual stress due to thermal shrinkage (~ 11 MPa) and pressure developed during impact (several GPa, depending on impact velocity)
- ✓ Surface roughness is in the order of nanometer scale. Combined effects of pressure and roughness is not well understood and needs to be investigated

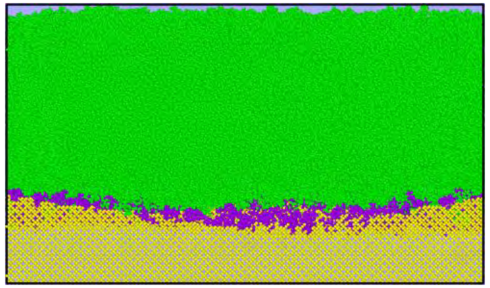


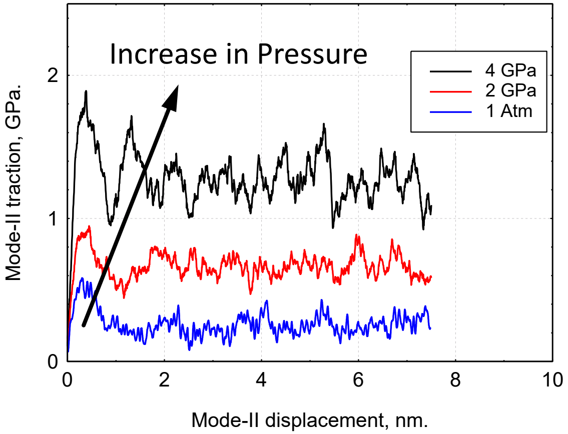
Ref.: C. Meyer et al.



Experimental (AFM) Profile of Glass Fiber Surface(Kubota et al.)







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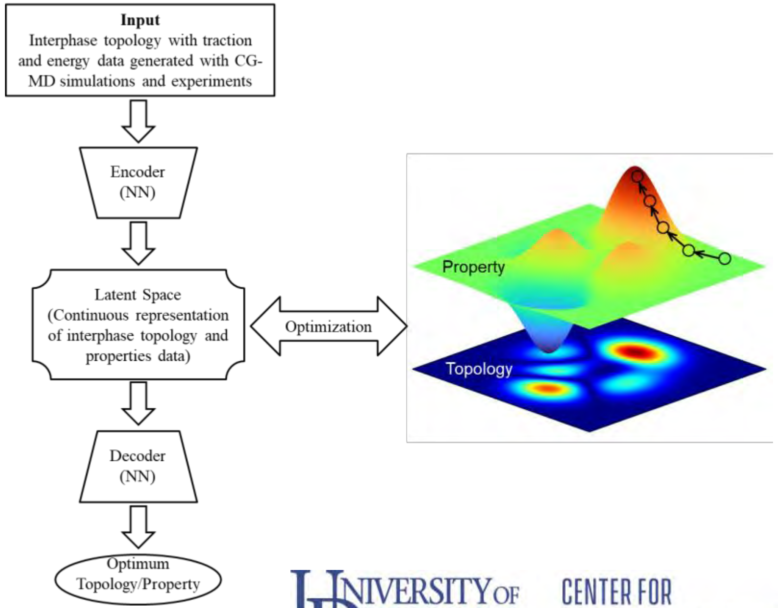
Transitions (materials, codes/tools, legacy publications)

- ✓ 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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