Multi-Scale Modeling of Fiber-Matrix Interphase (Fiber Modeling)

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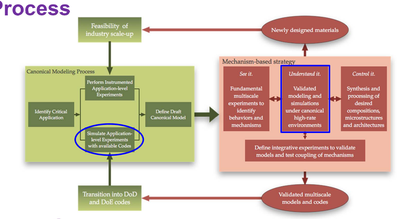
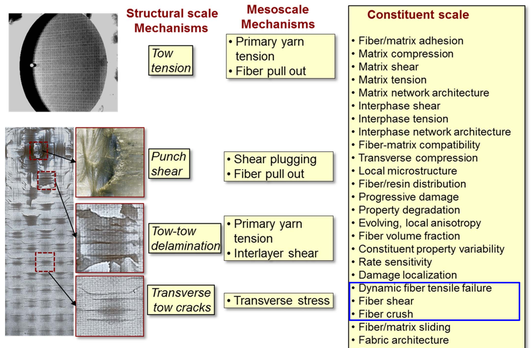
Enterprise for Multi-scale Research of Materials

How We Fit

Materials-by-Design Process



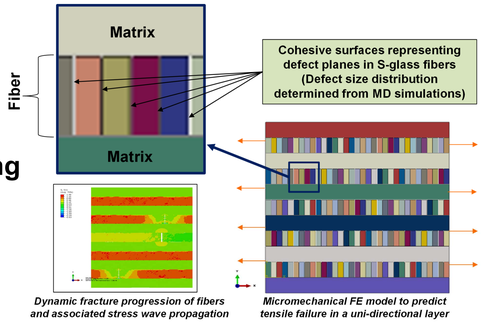
Mechanism-based Approach



Key Goals

- To improve computational efficiency, develop hybrid MD methodology to incorporate multiple potentials
- Apply this hybrid computational scheme in glass fiber modeling to determine
  - ✓ Cohesive traction law
  - ✓ Statistical strength distribution
  - ✓ Fracture energy release rate

- Apply this hybrid computational scheme in interphase modeling to develop traction law



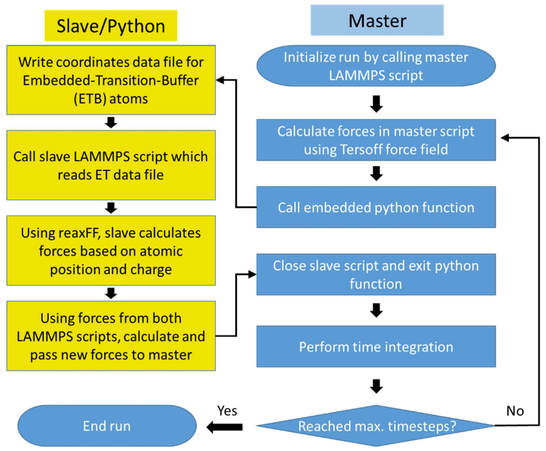
Dynamic fracture progression of fibers and associated stress wave propagation

Micromechanical FE model to predict tensile failure in a uni-directional layer

FE Based Micro-Mechanical Modeling of Composites

Technical Approach

- ✓ **Hybrid scheme will couple two or more force fields within LAMMPS-Python interface framework.**
- ✓ **Critical damage prone regions will be modeled by the ReaxFF**
- ✓ **Far field regions will be modeled by the cheaper (and/or non-reactive) force fields like Tersoff or AMBER.**

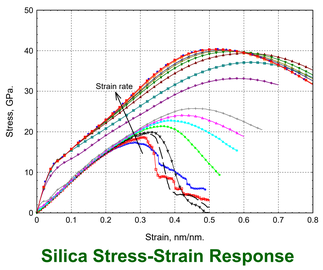


Flowchart of Lammps-Python interfacing for hybrid scheme

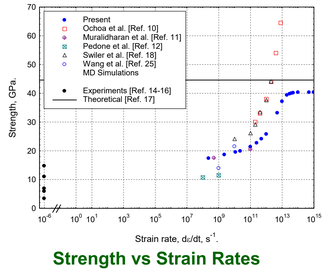
Major Results/Key Accomplishments

Fiber Modeling with Pure ReaxFF

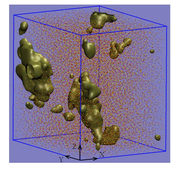
- ✓ **ReaxFF can better predict the structure and mechanical properties of silica glass**
- ✓ **ReaxFF is computationally expensive**
- ✓ **Hybrid scheme will reduce the computational cost**

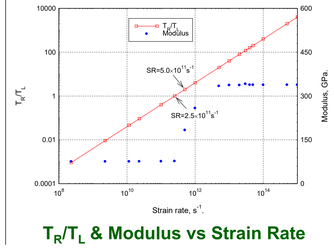


Silica Stress-Strain Response

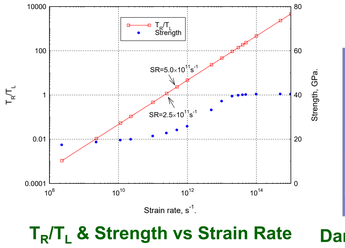


Strength vs Strain Rates

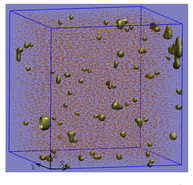




T_R/T_L & Modulus vs Strain Rate



T_R/T_L & Strength vs Strain Rate

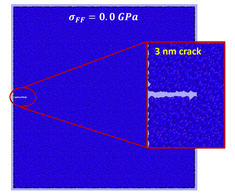


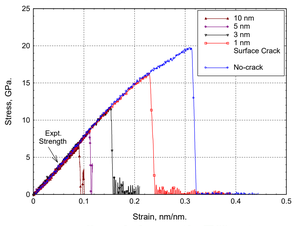
Damage Mode at High SR

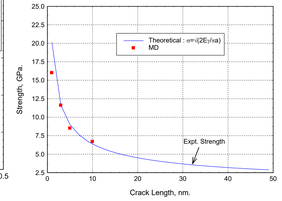
Major Results/Key Accomplishments

Surface Crack Modeling with Pure ReaxFF

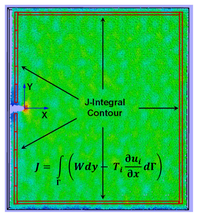
- ✓ **Determine statistical strength dist., fracture energy release rate**
- ✓ **Develop cohesive traction-separation law**
- ✓ **These information will be used in continuum level modeling**



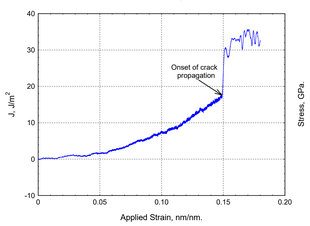




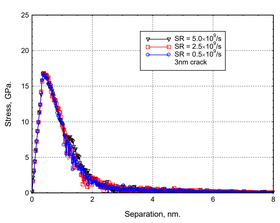
Crack Length Effects



J-Integral Contour

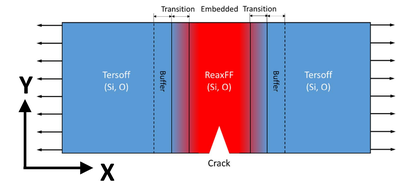


Variation of J with Strain

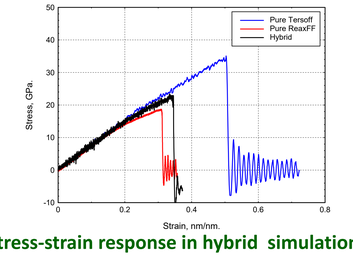


Cohesive Traction-Separation

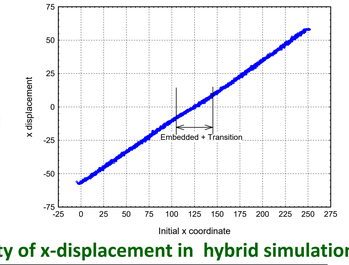
Hybrid Simulation: ReaxFF with Tersoff



- ✓ **Coupling Tersoff and ReaxFF force fields in the hybrid scheme yields accuracy of ReaxFF with less computational cost**
- ✓ **For 150000-atom model, hybrid simulation requires 8X less time compared to pure ReaxFF simulation**
- ✓ **Hybrid scheme maintain displacement continuity in the embedded-transition region boundary**



Stress-strain response in hybrid simulation



Continuity of x-displacement in hybrid simulation

Transitions/Impact

- ✓ **Hybrid MD scheme significantly improves computational efficiency**
- ✓ **MD predicted fiber properties will be used in continuum level composites micro-mechanics modeling**

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