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

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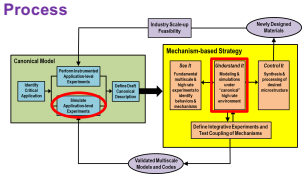
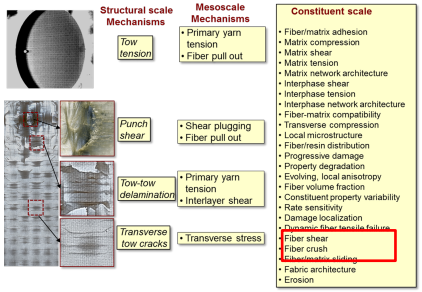
Enterprise for Multi-scale Research of Materials

How We Fit

Materials-by-Design Process

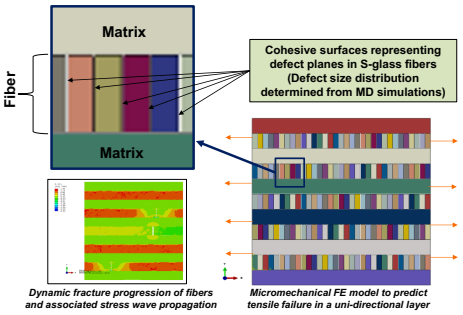


Mechanism-based Approach



Key Goals

- Study the strength improving mechanism of glass fibers
- Through molecular dynamics modeling, determine
  - ✓ Cohesive traction law
  - ✓ Statistical strength distribution
  - ✓ Fracture energy release rate



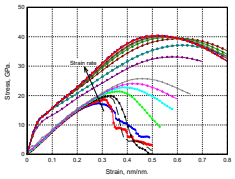
FE Based Micro-Mechanical Modeling of Composites

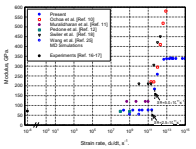
Technical Approach

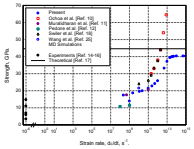
- Conduct molecular dynamics simulations to asses the capability of ReaxFF to predict the structure and mechanical properties of glass fibers
- Study the effects of cooling rate and temperature effects on glass properties
- Using glass model with surface crack, determine
  - ✓ Cohesive traction law
  - ✓ Statistical strength distribution
  - ✓ Fracture energy release rate

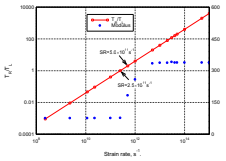
Major Results/Key Accomplishments

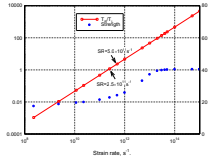
- ReaxFF can better predict the properties of silica glass compared to other reactive force fields

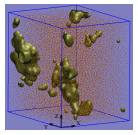

Silica Stress-Strain Response

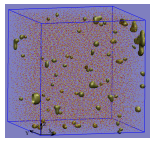

Modulus vs Strain Rates


Strength vs Strain Rates


Tr/Tl & Modulus vs Strain Rate


Tr/Tl & Strength vs Strain Rate

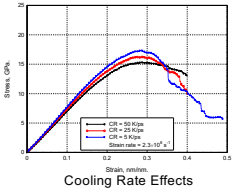

Damage Mode at Low SR

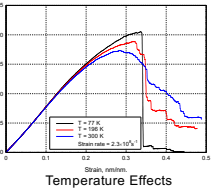

Damage Mode at High SR

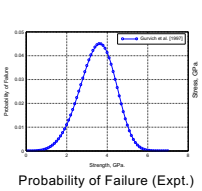
- Low strain rate loading allows sufficient time for voids growth and damage localization leading to lower bound on stress-strain response

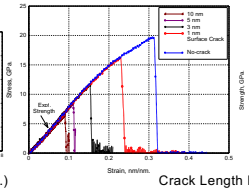
Major Results/Key Accomplishments

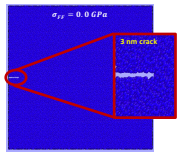
- Low cooling rate & low temp give higher mechanical properties

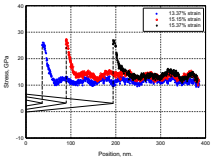

Cooling Rate Effects


Temperature Effects


Probability of Failure (Expt.)

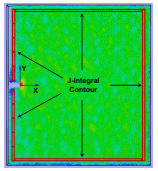

Crack Length Effects

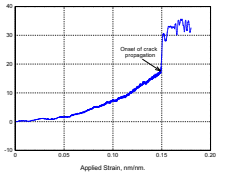

Stress Concentration at Crack Tip


Stress Variation in Front of Crack Tip

- Nano-meter size surface cracks significantly reduce strength
- J-Integral:

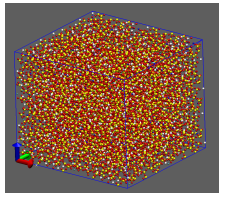
$$J = \int_{\Gamma} \left(W dy - T_i \frac{\partial u_i}{\partial x} d\Gamma \right)$$


J-Integral Contour


Variation of J with Strain

Future Directions in 2017

- Modeling of S-glass
  - SiO2 = 69%
  - Al2O3 = 22%
  - CaO = 5%
  - MgO=4%
- Modeling of crack healing mechanism with sizing
- Modeling of tensile fiber failure in presence of sizing/interphase


S-Glass Model

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