**Mechanism**

- Conduct molecular dynamics simulations to assess 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

**Materials**

- Fracture energy release rate and associated dynamic fracture progression of fibers determined from MD simulations.
- Cohesive surfaces representing defect phases in S-glass fibers (Defect size distribution determined from MD simulations).

**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

**Technical Approach**

- ReaxFF can better predict the properties of silica glass compared to other reactive force fields.
- Nano-meter size surface cracks significantly reduce strength.
- J-Integral:
  \[ J = \int_{\Gamma} (\sigma - T unn) \cdot dA \]

**Major Results/Key Accomplishments**

- Low cooling rate & low temp give higher mechanical properties.
- Modulus vs Strain Rates.
- Strength vs Strain Rates.
- Damage Mode at Low SR.
- Damage Mode at High SR.

**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.