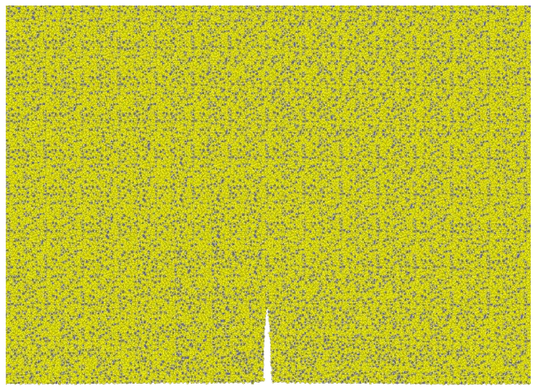
ATOMIC LEVEL STRESS ANALYSIS IN GLASS FIBERS

Tim B. Longoria (B.Ch.E.), Dr. Sanjib C. Chowdhury, and Prof. John W. Gillespie Jr.
University of Delaware | Center for Composite Materials

Introduction

- Glass fibers are used in optical fibers and in structural reinforcing composite materials.
- It is important to understand the effects of surface defects on the mechanical properties of glass fibers and to determine the fracture toughness of glass fibers.

Silica Glass MD Model with 10nm Crack



Problem Specification

- During glass fiber spinning and handling operations, surface cracks on a nanometer scale appear.
- It is thought that the surface cracks reduce the glass fibers' strength, but the small scale makes experimental observation difficult to prove that.
- Molecular dynamics (MD) simulations with reactive force field ReaxFF are used to study the effects of surface crack on the mechanical properties of glass fiber at this small length scale.

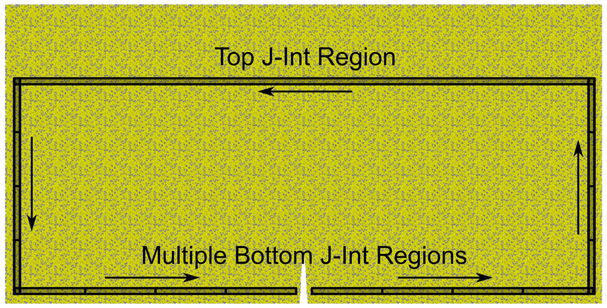
Methodology

- Fracture toughness is determined using atomistic J-integral approach.

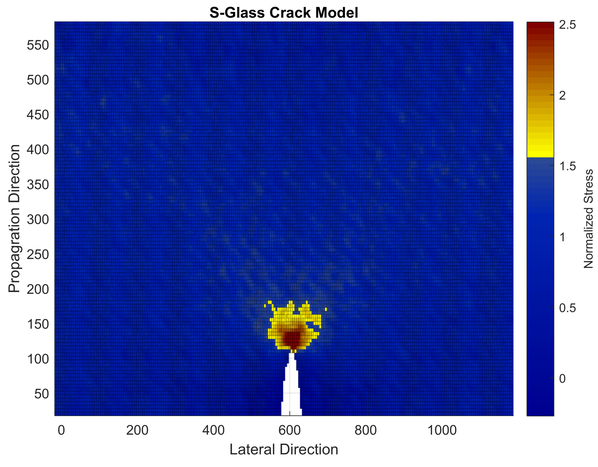
$$J = \int_{\Gamma} (W dx - T_i \frac{\partial u_i}{\partial y} d\Gamma)$$

$$W = \frac{1}{2}(\sigma_x \varepsilon_x + \sigma_y \varepsilon_y + \sigma_{xy} \varepsilon_{xy})$$

[Chowdhury et. al., Engg. Fract. Mech., 207, 2019]

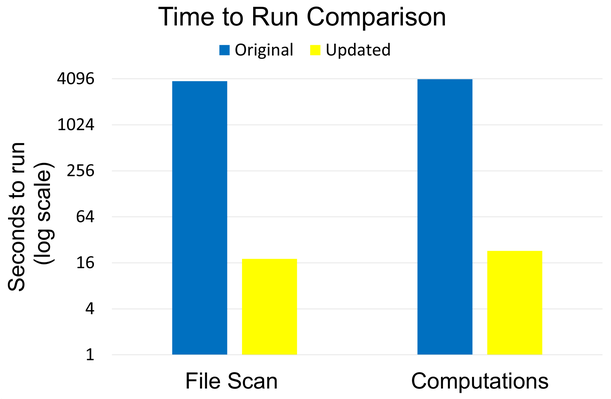


- This requires to calculate continuum level equivalent Hardy stress (σ) from the atomic stress obtained from MD simulation.
- Matlab scripts are developed to calculate Hardy stress.
- As expected, Hardy stress shows stress concentration in front of crack tip.
- Hardy stress is visualized by sorting atoms into position-based boxes and averaging the respective stress values.

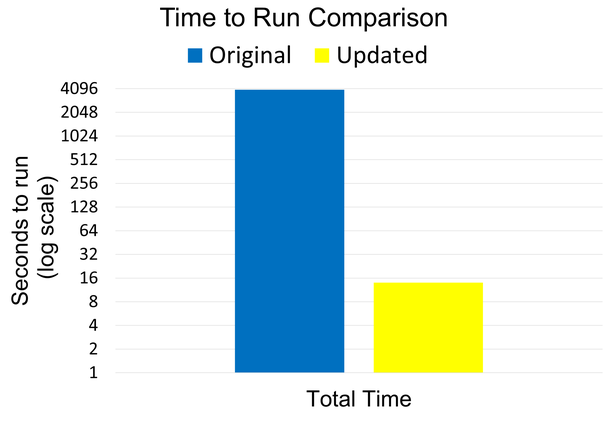


Results and Discussion

- Significant increase in processing speed between multiple scripts by converting large loops with Matlab vectorization.
- Vectorized Matlab code takes advantage of parallelism to increase speed as well as create shorter and more readable code.
- The updated Hardy stress script resulted in a 99% decrease in time to run.

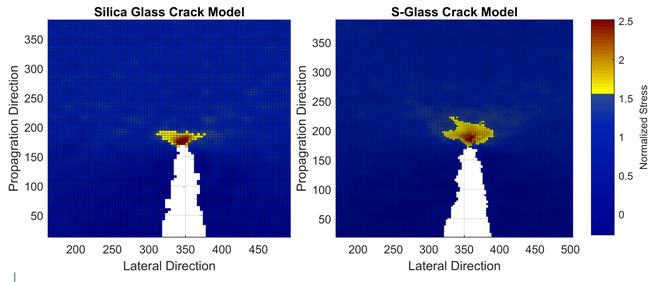


- Engineering stress calculation script resulted in a 99.7% decrease in time to run

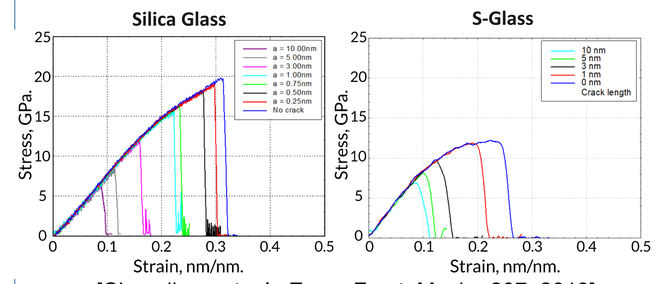


Summary and Conclusion

- Molecular dynamics simulations are useful for studying fracture mechanism and surface crack impact on glass fibers' (silica glass and s-glass) mechanical properties.
- The simulations shows that large size cohesive zone develops in front of the crack tip in case of S-glass indicating S-glass is more ductile compared to silica glass.
- The crack propagates and grows as the molecular bonds break.



- Crack significantly reduces the strength of the fiber without affecting modulus



[Chowdhury et. al., Engg. Fract. Mech., 207, 2019]

Acknowledgements

Tim would like to acknowledge the internship supported by the US Army through the Undergraduate Research Apprenticeship Program (URAP)

Co-Sponsored by:
University Leadership Initiative (ULI)
Partner