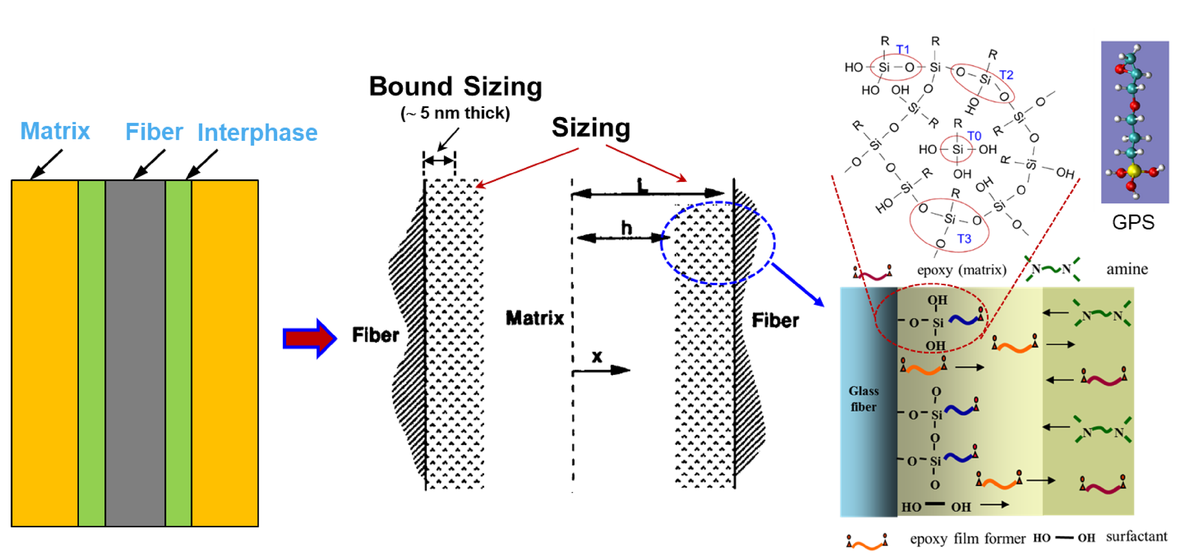
Strain Rate Dependent Cohesive Traction Laws for Glass Fiber-Epoxy Interphase using Molecular Dynamics Simulations

UNIVERSITY OF DELAWARE | CENTER FOR COMPOSITE MATERIALS

Dr. Sanjib C. Chowdhury & Prof. John W. Gillespie, Jr.
University of Delaware | Center for Composite Materials

Introduction

- In the glass fiber-epoxy composite, interphase is a distinct region between fiber and epoxy matrix that develops during processing through diffusion and reaction between the matrix and the fiber sizing
- Interphase could have different morphology depending on processing and thickness could vary from few nanometers to tens of nanometers
- Since load is transferred through interphase, it controls composites strength, toughness, and damage modes
- In high-velocity impact, interphase could be subjected up to 1e12/s strain rate, and like many other materials interphase properties are also strain rate dependent
- Therefore, it is essential to understand the interphase properties tailoring mechanism at the atomistic scale as well as its strain rate-dependent responses



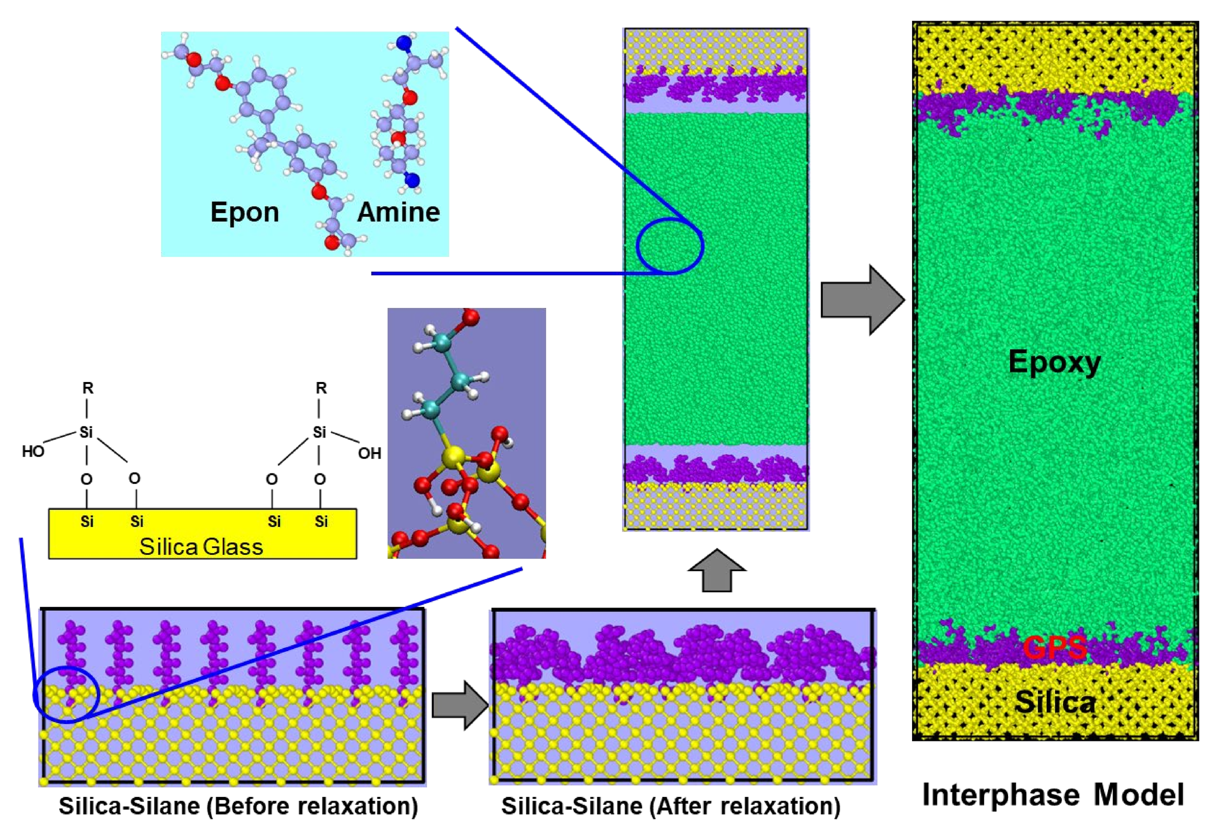
Fiber-Matrix Interphase System

Objectives

- Establish a molecular dynamics (MD) based "Materials-by-Design" framework for composite interphase
- Develop strain-rate dependent traction law to bridge length scales in the finite element (FE) based continuum level micro-mechanics modeling of composites

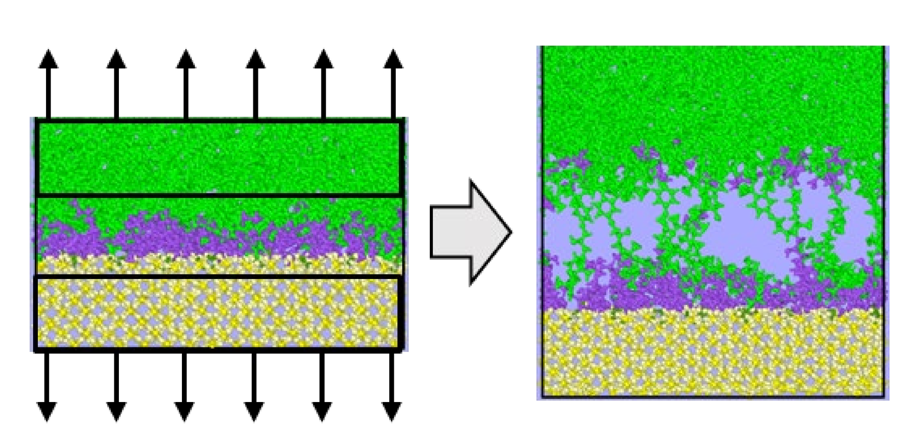
Simulations Details

- We develop fiber-epoxy interphase with mono-layer 3-glycidoxypropyltrimethoxy silane (GPS)
- First, we deposit hydroxylated mono-layer silane on the silica surface at different number densities (0/nm^2 to 3.9/nm^2) and react them with the silica surface through condensation reaction
- In the second step, a mixture of the Epon828-Jeffamine® D-230 is put on the silica slab, equilibrated, and cured
- Condensation and curing reaction are modeled with AMBER based cross-linking algorithm
- The model is then equilibrated with reactive force field ReaxFF before being subjected to mechanical loading



Interphase Model Development Procedure

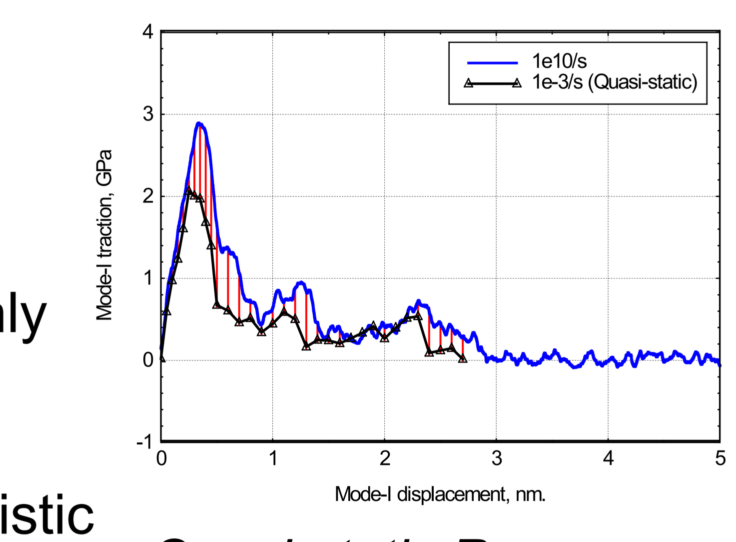
- Interphase thickness is determined from the Root Mean Squared Fluctuation method
- Interphase thickness is in the range of 1.3 to 1.7 nm for mono-layer silane



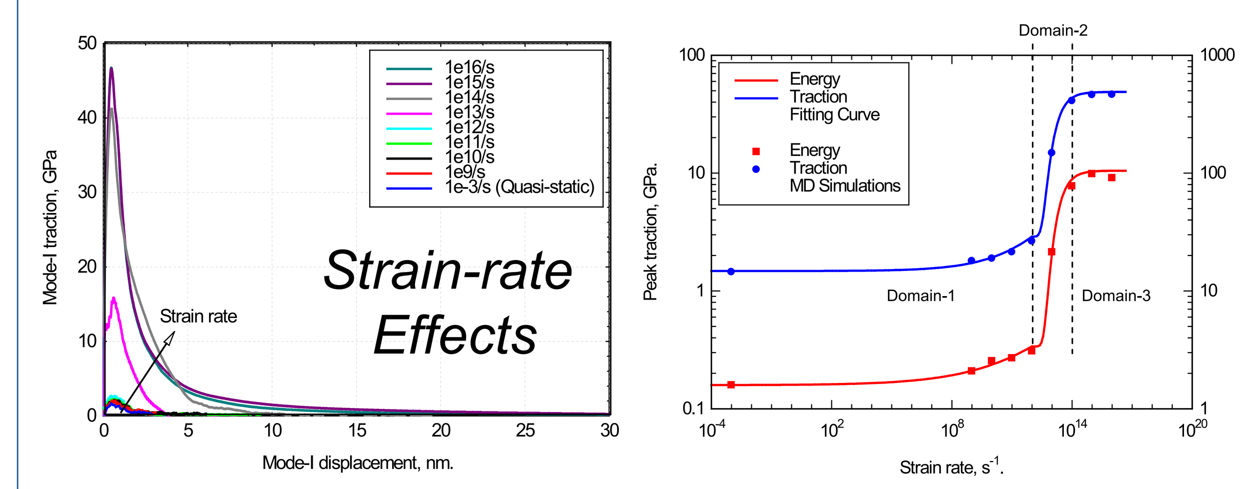
Mode-I Loading

Results and Discussion

- Interphase is loaded in Mode-I at strain rates 1e9/s to 1e16/s including quasi-static loading
- Quasi-static response is determined from the tens of relaxation simulations at different deformation states
- Irrespective of interphase topology, peak traction and energy are highly strain-rate dependent and show characteristic S-shape response



Quasi-static Response



- We successfully established the correlation between peak traction and energy as a function of silane number density and strain rate with the following equations.

Peak Traction:

$$T =[T_{0,QS}(1+a_T*D_{SN})][1 + b_T\dot{\varepsilon}^{c_T}], \text{ for } \dot{\varepsilon} \leq 1e12/s \quad (1a)$$

$$T =[T_{0,QS}(1+a_T*D_{SN})]\left[1 + b_T\dot{\varepsilon}_{1,T}{}^{c_T}\right] + [g_T + h_T * D_{SN}]exp\left(-(m_T - n_T * D_{SN})\dot{\varepsilon}/\dot{\varepsilon}_{2,T}\right), \text{ for } \dot{\varepsilon} > 1e12/s \quad (1b)$$

Energy:

$$G = \left[G_{0,QS}\left(a_{1,G} - (a_{1,G} - a_{2,G})exp(-D_{SN}/a_{3,G})\right)\right][1 + b_G\dot{\varepsilon}^{c_G}], \text{ for } \dot{\varepsilon} \leq 1e12/s \quad (2a)$$

$$G = \left[G_{0,QS}\left(a_{1,G} - (a_{1,G} - a_{2,G})exp(-D_{SN}/a_{3,G})\right)\right]\left[1 + b_G\dot{\varepsilon}_{1,G}{}^{c_G}\right] + [g_G + h_G * D_{SN}]exp\left(-(m_G - n_G * D_{SN})\dot{\varepsilon}/\dot{\varepsilon}_{Ref,G}\right), \text{ for } \dot{\varepsilon} > 1e12/s \quad (2b)$$

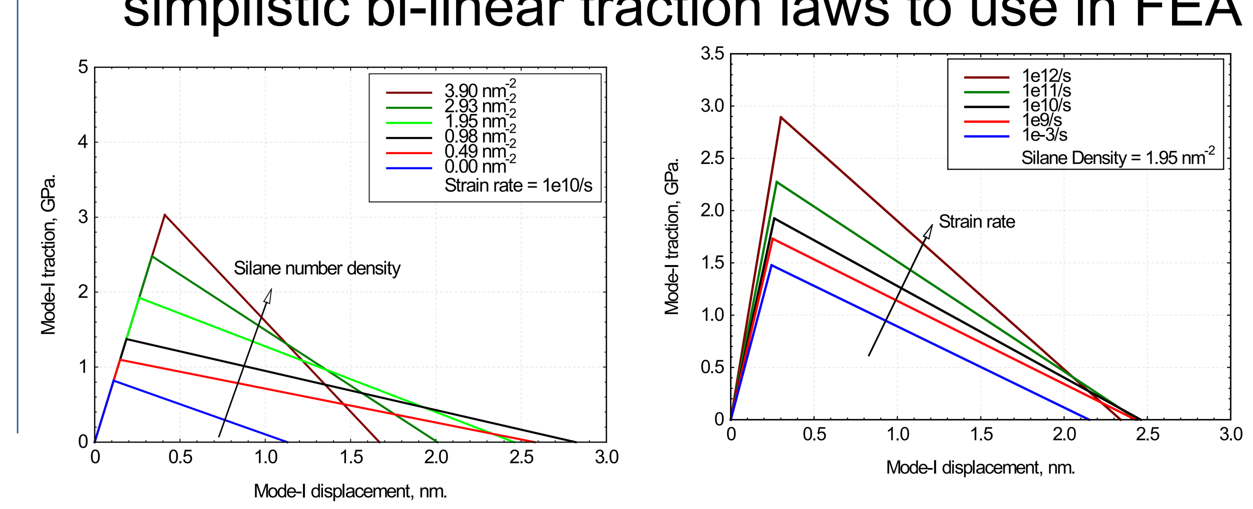
Stiffness:

$$K = \left[K_{QS} + a_K\dot{\varepsilon}^{b_K}\right], \text{ for } \dot{\varepsilon} \leq 1e12/s \quad (3a)$$

$$K = \left[K_{QS} + a_K\dot{\varepsilon}_{1,K}{}^{b_K}\right] + c_K exp\left(-\dot{\varepsilon}/\dot{\varepsilon}_{2,K}\right), \text{ for } \dot{\varepsilon} > 1e12/s \quad (3b)$$

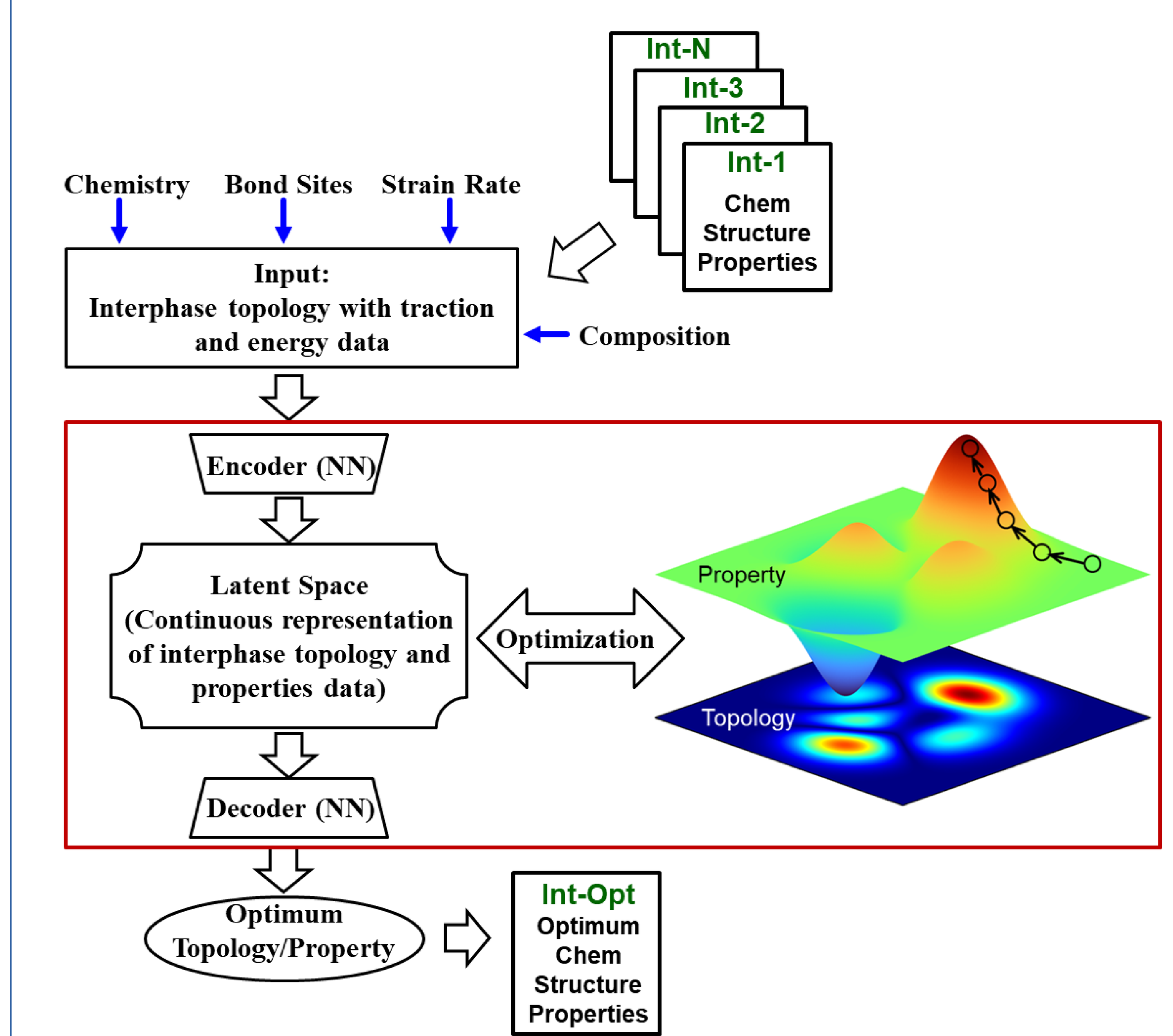
T is the traction, G is the energy, $\dot{\varepsilon}$ is the strain rate, D_{SN} is the silane number density, $T_{0,QS}$ and $G_{0,QS}$ are the quasi-static traction and energy for the interphase without silane.

- The above correlations are used to predict simplistic bi-linear traction laws to use in FEA



Path Forward

- We are in the process of developing strain-rate-dependent mixed-mode traction law
- Develop physics informed machine learning framework to design composite interphase for optimum strength and energy considering variability in interphase chemistry, topology, and strain rate



References

- Chowdhury et al., Glass fiber-epoxy interactions in the presence of silane: A molecular dynamics study, Applied Surface Science 2021, 542:148738
- Chowdhury et al., Strain-Rate Dependent Mode I Cohesive Traction Laws for Glass Fiber-Epoxy Interphase using Molecular Dynamics Simulations. Composites Part B 2022, 237:109877

Acknowledgements

This work is supported by the Army Research Laboratory through the Materials in Extreme Dynamic Environment (MEDE) program.