ATOMISTIC ANALYSIS OF INTERPHASE AND POLYETHLYENE FIBERS

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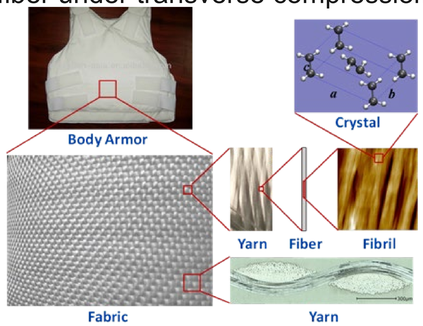
Introduction

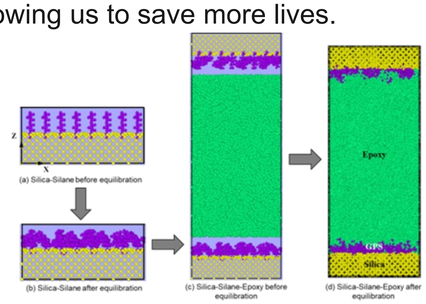
- In glass fiber-epoxy composite materials, interphase is the region in-between fiber and matrix which develops through diffusion and reaction during composite manufacturing
- Polyethylene (PE) fibers are light weight materials that offer enhanced strength and energy absorption
- Using molecular dynamics (MD) simulations we analyze the performance of composite interphase as well as PE fibers

Develop pre- and post-processing tools to (a) create/analyze composite interphase (b) assess change in structure of PE fiber under transverse compression



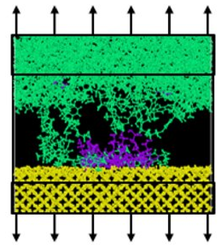
Problem Specification

- Improving the interphase in glass-epoxy composites will allow for a wider variety of uses as it controls strength and toughness in the material.
- Better PE fibers can offer soldiers more resistance to bullets and shrapnel, allowing us to save more lives.

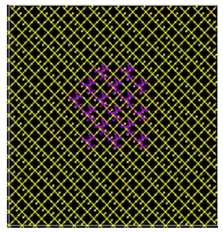


Methodology

- Develop composite interphase model with defects (i.e., agglomerated silanes on fiber surface)

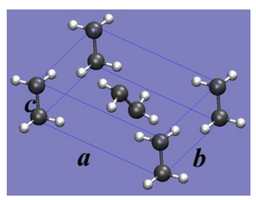


Mode-I interphase loading



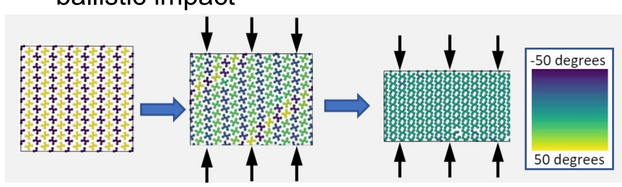
Agglomerated silane on surface

- Previously simulations used fiber substrate with uniformly distributed silanes. Now we are looking into effects of irregularities in silane deposition on the substrate
- To determine the stress–strain response and damage modes of the silica-epoxy composite, the silica-epoxy composite model is subjected to transverse tension and shear loading using ReaxFF
- The primary element of PE fibers are the crystal lattice



PE Crystal Unit Cell 3D Model

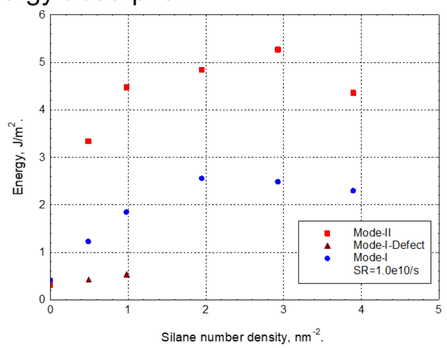
- Chains are aligned along the C-axis, interactions are non-bonded van der Waals in the lateral direction
- MATLAB scripts are used to track the change in morphology during ballistic impact



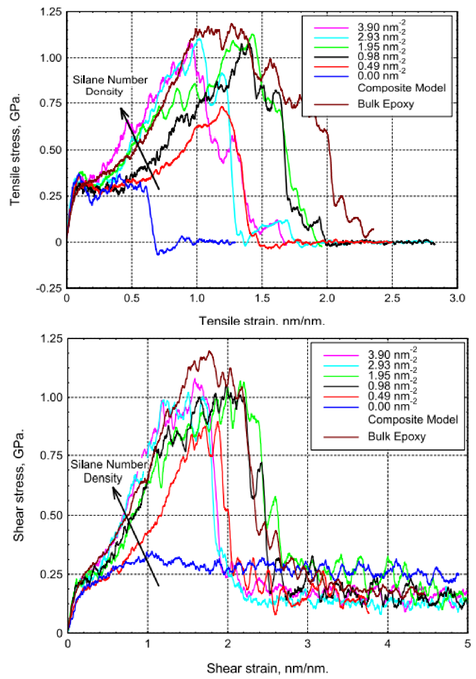
Change in morphology in polyethylene (PE) crystal under transverse pressure (color coded based on the angle of the chains).

Results and Discussion (Interphase)

- A lot of work with interphase has already been done
- Defective interphase gives low energy absorption.



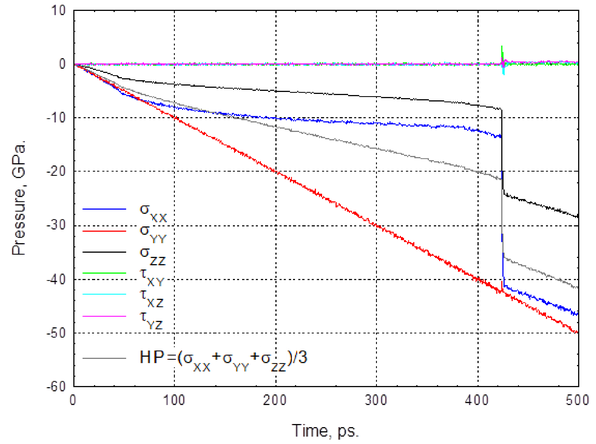
- As silane density increases, so does the energy absorption of the interphase



Chowdhury et al., Applied Surface Science, 542, 2021

- Tensile and shear strength also seem to increase as silane number density increases until around 1-2 nm^2

Results and Discussion (PE Fiber)



- Under transverse pressure, phase transformation (orthorhombic to monoclinic shown in methodology) occurs near 21.5 GPa hydrostatic pressure for polyethylene crystal

Summary and Conclusion

- Interphase properties improve as silane density and covalent-bonded interaction in the interphase region increase
- A silane number density of about 1-2 nm^2 is an optimal density for a silane-epoxy composite system regarding for both high strength and energy
- Simulations for the interphase with non-uniform silane are in progress
- MD simulations can capture the phase transformation of polyethylene crystal under transverse pressure
- More research needs to be done to understand the load transfer mechanism within the fiber at different length scales. MD simulations can be used to understand these mechanism

Acknowledgements

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