Modeling the Fibrillated Microstructure of UHMWPE Fibers

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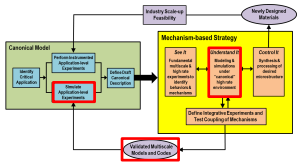
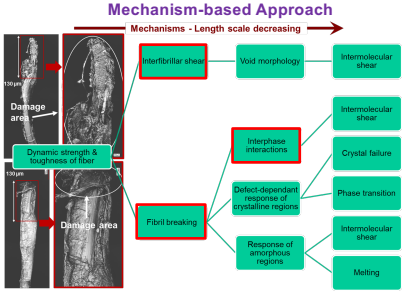
Enterprise for Multi-scale Research of Materials

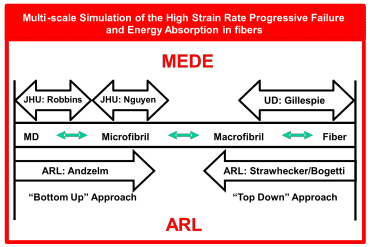
How We Fit

Materials-by-Design Process



Mechanism-based Approach



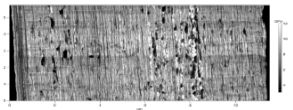


- Coordination and collaboration between MEDE and ARL Mission programs are essential in the development of a comprehensive multi-scale model for advanced UHMWPE fiber design

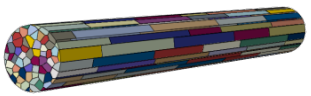
Key Goals

Significantly improve our fundamental understanding of the dominant mechanisms at sub-fiber length scales that govern the intrinsic macro-scale behavior of UHMWPE fibers

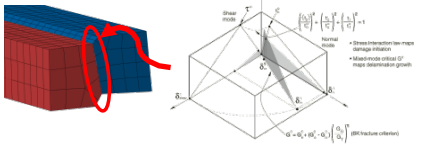
- Understand the internal fibrillated microstructure of UHMWPE fibers



- Develop a model representation of the microstructure to capture the deformation mechanisms of the fiber

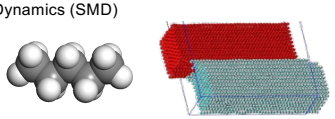


- Use the model to understand the role of the microstructure and guide new fiber development

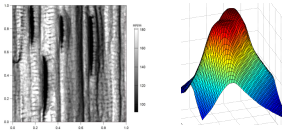


Technical Approach

- Material properties and inter-microfibril traction laws are calculated with Steered Molecular Dynamics (SMD)

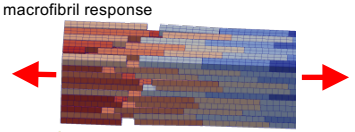


Microfibril/crystal length scale (10-100 nm)

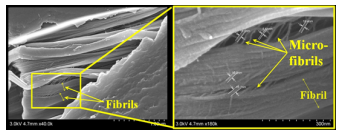


- Nano-indentation and scratching experiments measure the properties and interactions of microfibrils

- Finite element (FE) models at intermediate length scales use SMD predictions to simulate macrofibril response

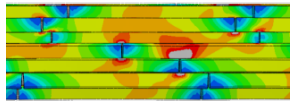


Macrofibril length scale (0.1-1 μm)

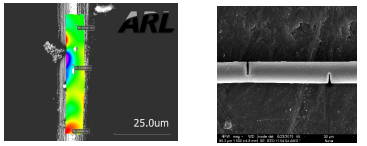


- Evaluation of the microstructure provides insights into the important mechanisms of interaction

- Heterogeneous fiber FE models are used to investigate macrofibril interactions and predict single fiber experiments



Fiber length scale (10-20 μm)

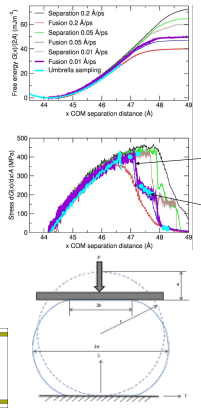


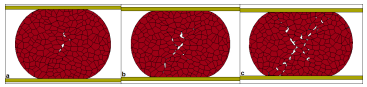
- Experimental results of single fiber testing to provide validation for modeling

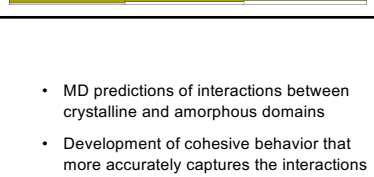
Major Results/Key Accomplishments

- Prediction of fibril surface interaction properties with free energy calculations by atomistic molecular dynamics (MD) simulations using both Steered MD (Jarzynski's identity) and Umbrella Sampling (US) simulations $e^{-\beta\Delta F} = \langle e^{-\beta W_t} \rangle$
- Consistent and complementary free energy/force profiles of fibril surface interactions were obtained from steered MD (SMD) and umbrella sampling (US) simulations
- Developed a heterogeneous fiber FE model to simulate fiber cross-section containing 250 macrofibrils
- Model used to predict nominal stress-strain response of single Kevlar fiber transverse compression

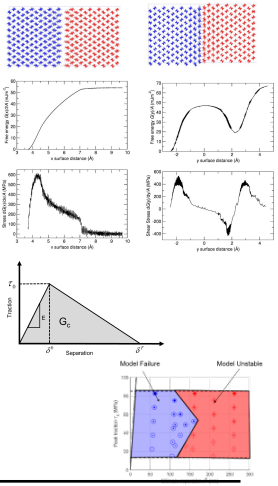
Free energy/force profiles





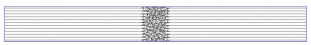


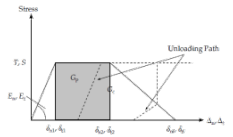
- Estimated surface free energy, 55-78 mJm^{-2}, are in agreements with experimental and theoretical predictions for van der Waals surfaces, 40-93 mJm^{-2}
- Free energy/force profiles with respect to surface distance display clearer pictures of fibril surface interactions
- The estimated maximum shear stress, 514 MPa, is similar to that from shear deformation simulation
- Parametric study conducted on the peak traction and ultimate separation of a bilinear cohesive zone model
- Cohesive energies ranged from 0.8-10 Jm^{-2}, largest stable energy of 4.2 Jm^{-2} predicted fiber failure
- Experimental measurements of macrofibril interactions range from 10-20 Jm^{-2}
- Additional energy absorbing mechanisms are required to capture macrofibril interactions



Future Directions in 2017

- MD predictions of interactions between crystalline and amorphous domains
- Development of cohesive behavior that more accurately captures the interactions in the fiber's microstructure





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