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Modeling fibrillation as an energy absorbing mechanism in the transverse compression response of fibers

ARL

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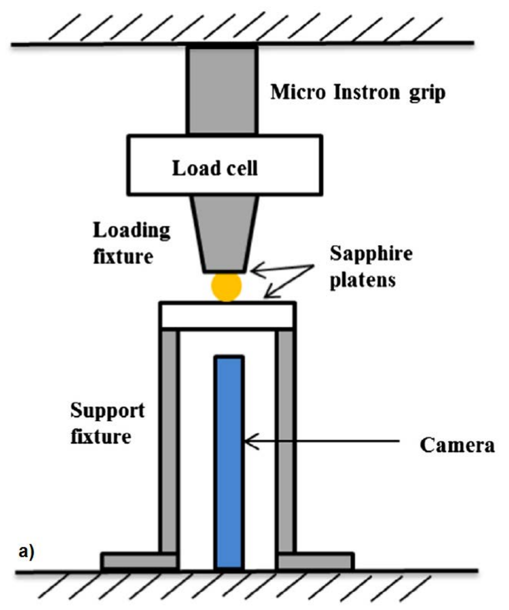
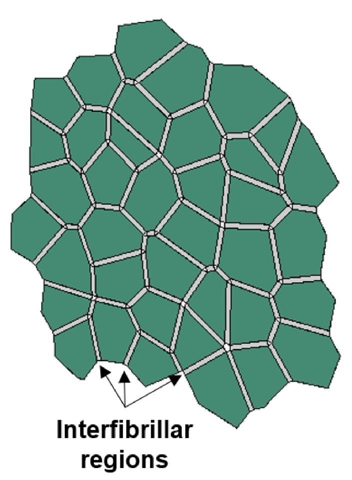
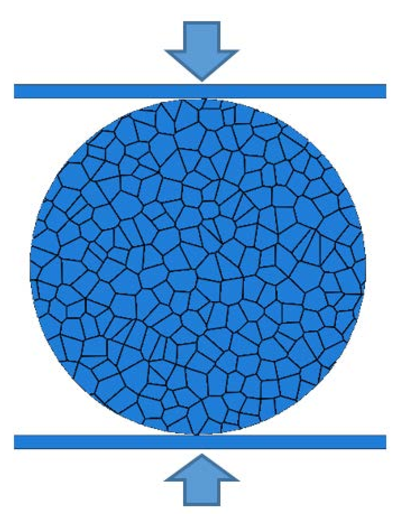
Enterprise for Multi-scale Research of Materials

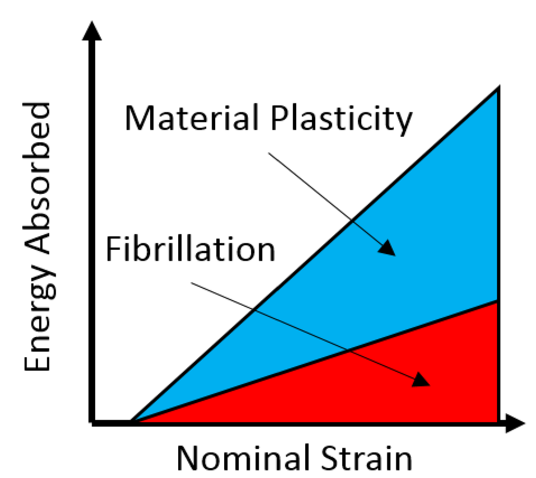
Modeling Approach

- Developed a heterogeneous fiber FE model to simulate fiber cross-section containing 250 macrofibrils
- Fibrillation mechanisms introduced through interfibrillar response (cohesive traction-separation behavior)
- Model used to predict nominal stress-strain response of single Kevlar fiber in transverse compression



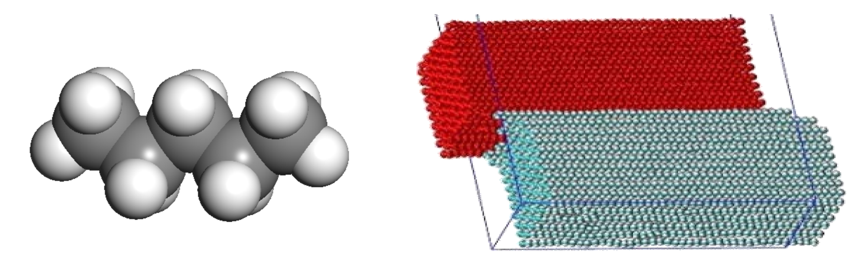




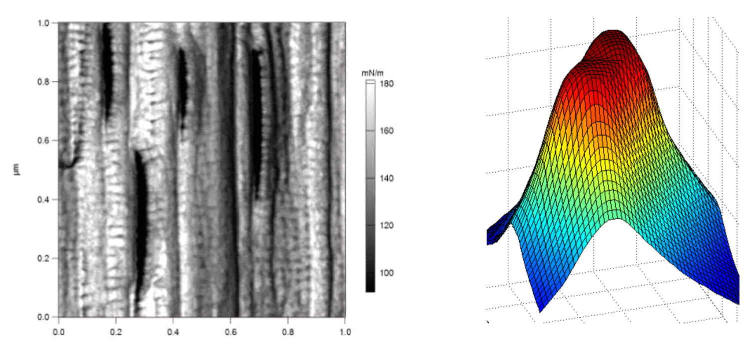


Multiscale Modeling and Experiments

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

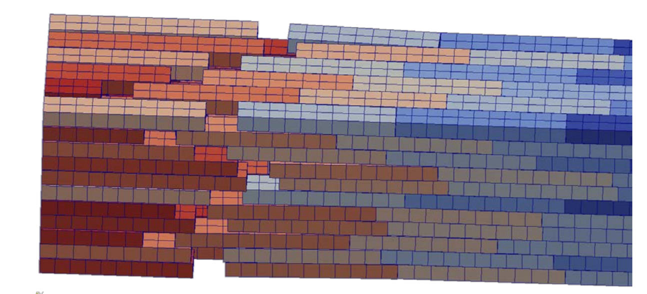


Microfibril/crystal length scale (10-100 nm)

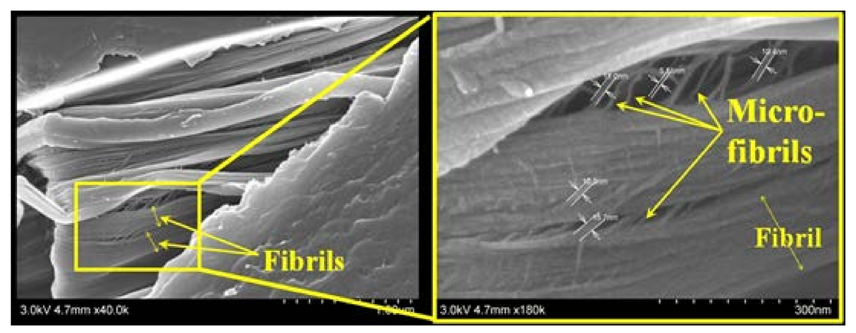


- Nano-indentation and scratching experiments measure the properties and interactions of microfibrils

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

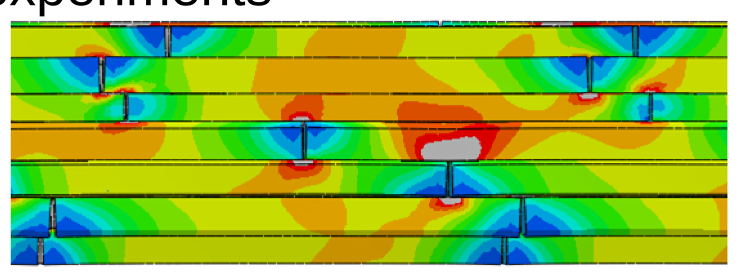


Macrofibril length scale (0.1-1 μm)

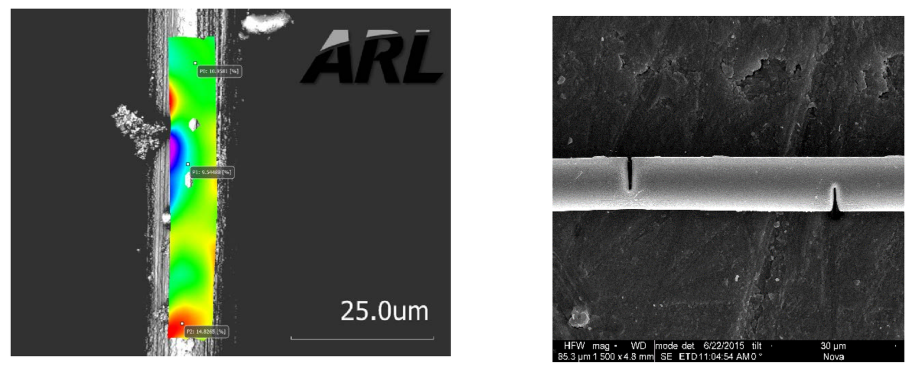


- Evaluation of the microstructure provides insights into the important mechanisms of interaction

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



Fiber length scale (10-20 μm)

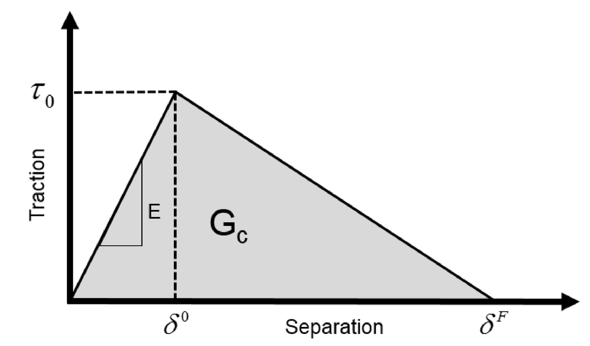


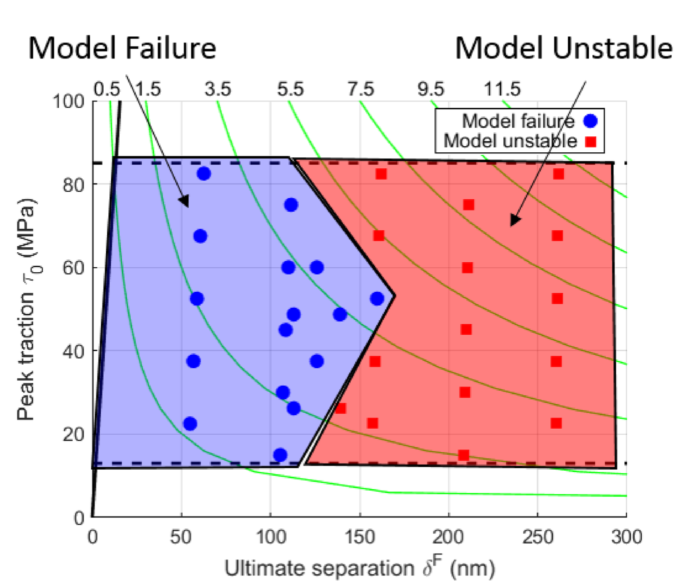
- Experimental results of single fiber testing to provide validation for modeling

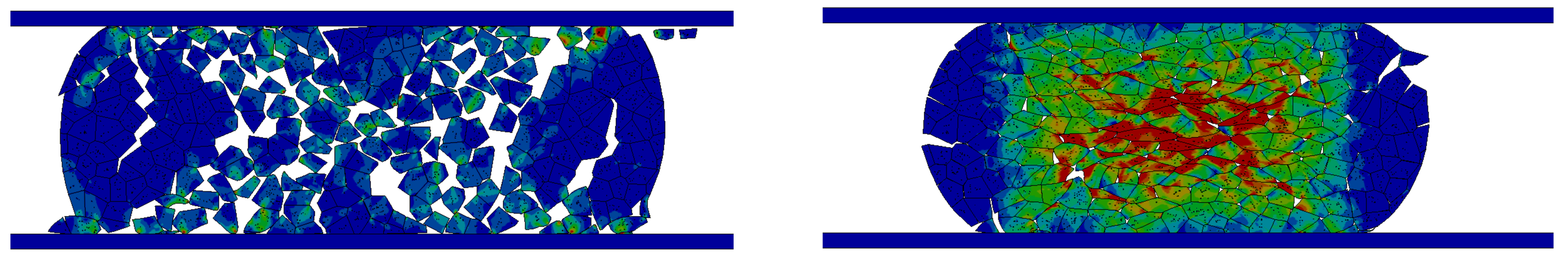
Major Results/Key Accomplishments

Uniform Distribution

- 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

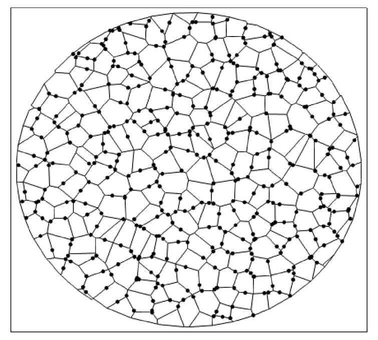


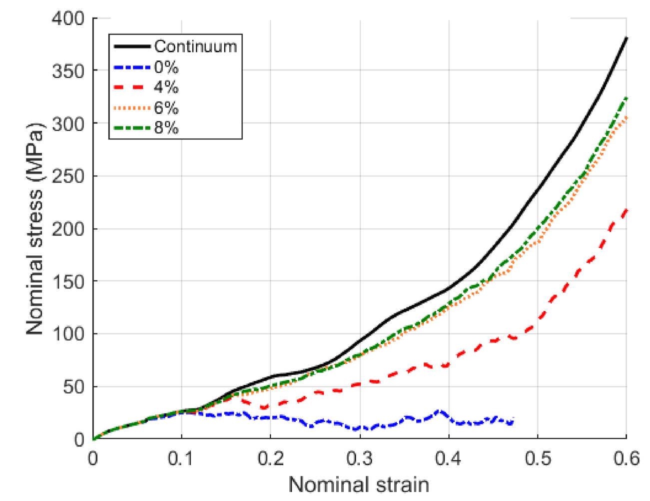


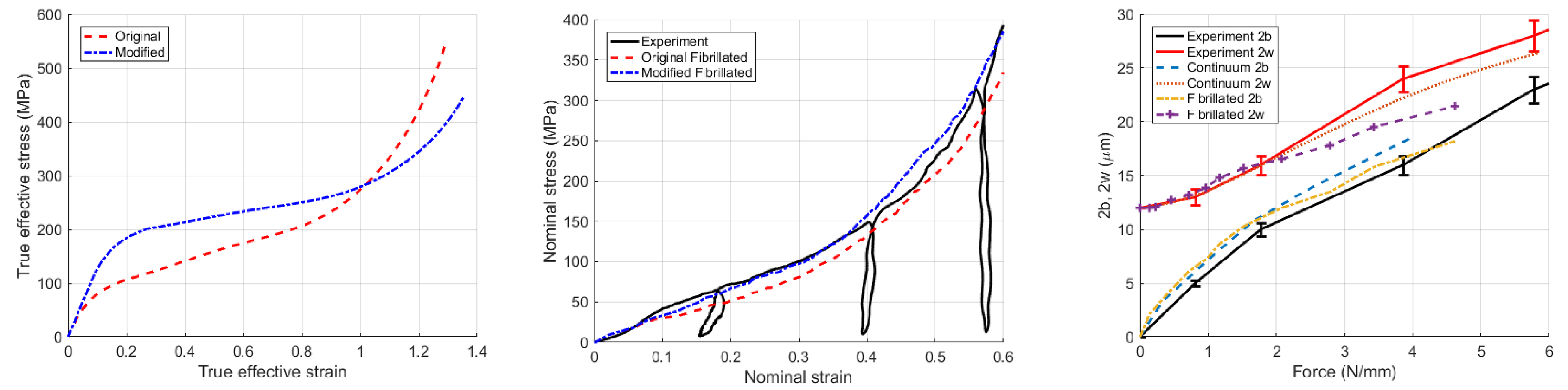


Bi-modal Distribution

- A small amount of strong interactions significantly effects the predicted transverse compressive response
- Strong interactions represent bridging microfibrils and tie chains, reflecting networked microstructure
- With compliance introduced through fibrillation, yield stress of transverse macrofibril response is increased to correlate to experimental results
- Contact width predictions improve upon continuum predictions, although fiber width expansion is underpredicted



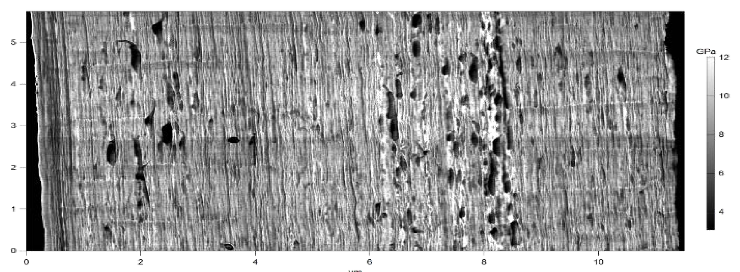




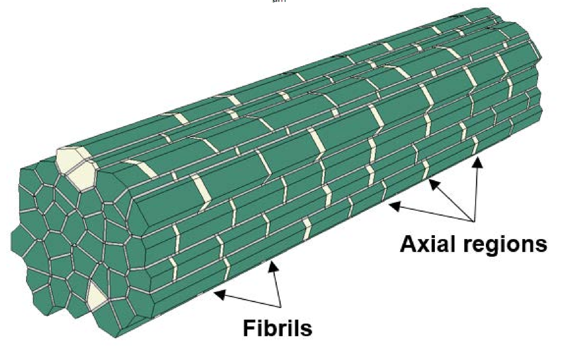
Long Term Goals

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

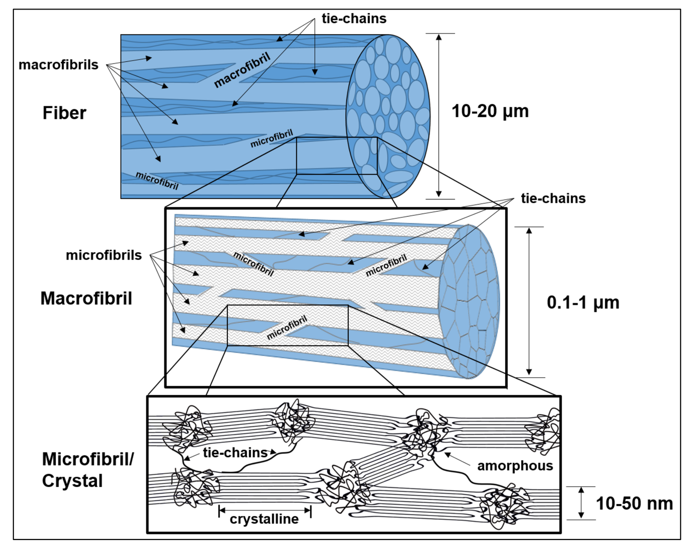
- Understand the internal fibrillated microstructure of UHMWPE and Kevlar fibers



- 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



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