MOLECULAR DYNAMICS STUDY OF THE EFFECTS OF DEFECTS AND TRANSVERSE PRESSURE ON THE AXIAL TENSILE PROPERTIES OF POLYETHYLENE

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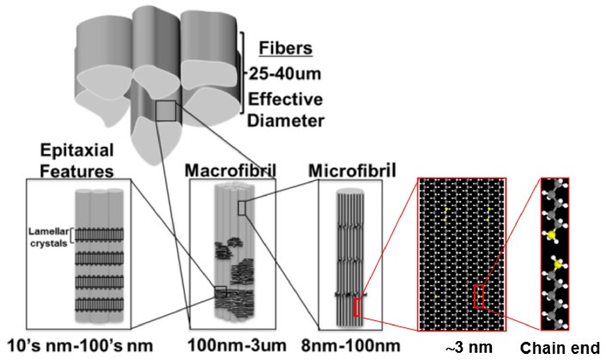
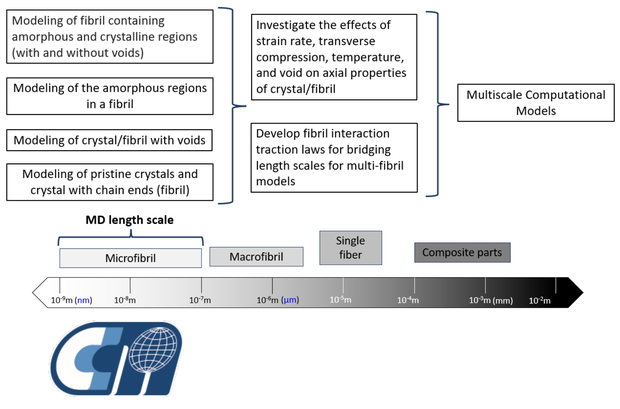
Introduction

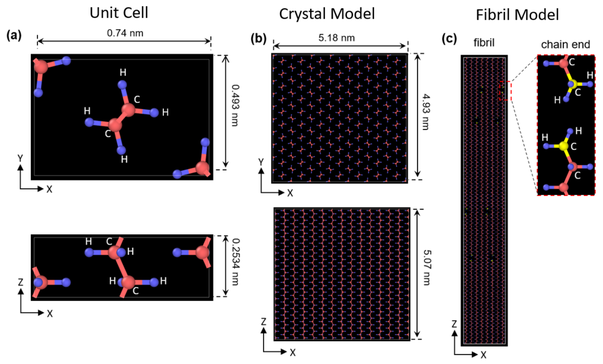


- UHMWPE fiber with a diameter of 25-40 μm is comprised of thousands of fibrils and total void content in the range of 20-30%.
- During a ballistic impact, these porous fibers within the laminates undergo significant transverse pressure and axial tension.
- The influence of transverse pressure and voids on the mechanical properties of PE fibers remains poorly understood.
- To address this knowledge gap, we employ molecular dynamics simulations to investigate the behavior of porous polyethylene structures under transverse pressure.

Overall Modeling Approach

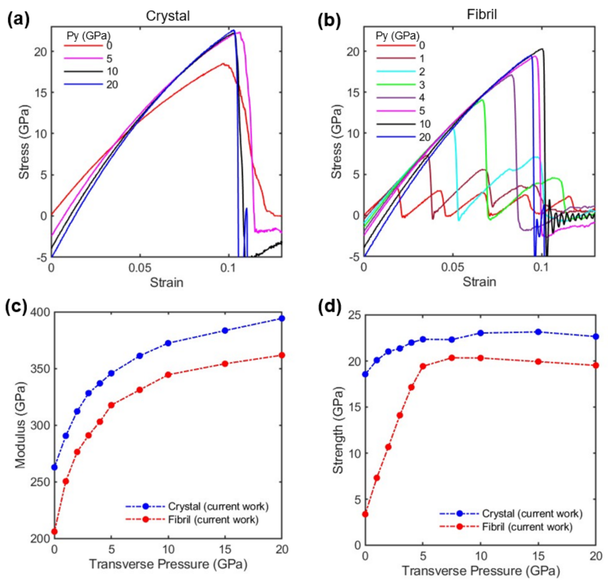


Molecular Dynamics Models



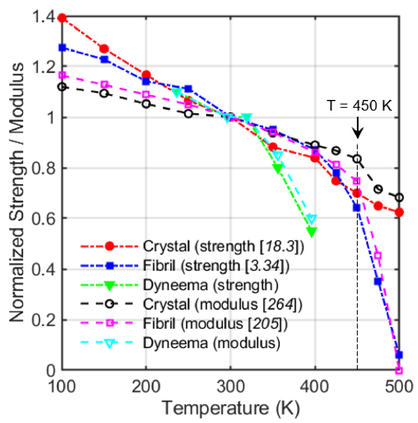
- LAMMPS with AIREBO-M potential to was used for the simulations.

Effect of Transverse Pressure



- Five-fold increase in the strength of fibril was observed due change in the failure mode from chain sliding to chain scission.

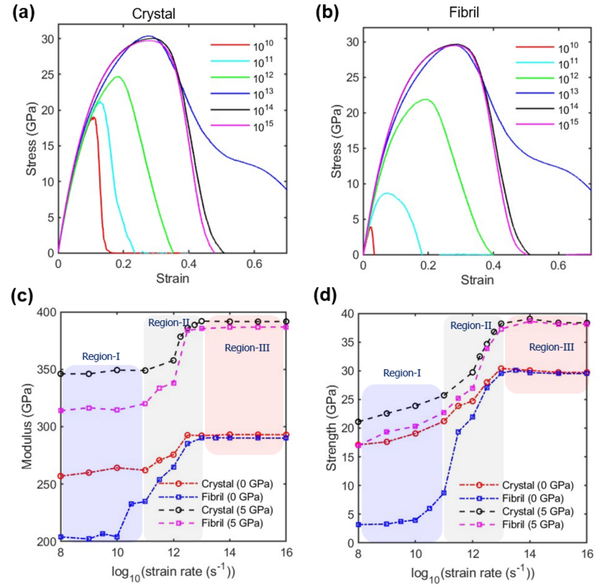
Effect of Temperature



The values have been normalized relative to their corresponding values at 300 K, which are given in the legend.

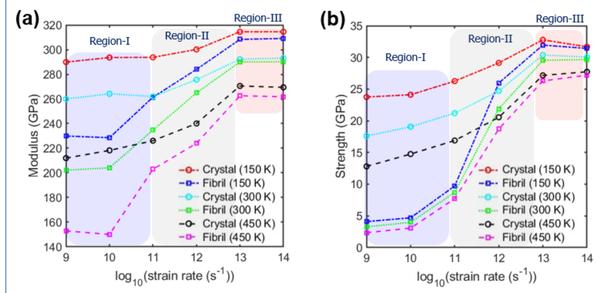
- Simulations reveal that the melting temperature of PE crystal is ~450 K.

Effect of Strain Rate & Pressure



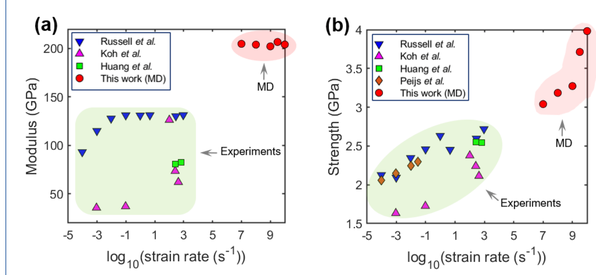
- The jump in strength & modulus of fibril is due to the transition of the failure mode from chain sliding to chain scission, which happens when the loading rate exceeds the chain sliding velocity.

Effect of Strain Rate & Temperature



- Material properties improve with decreasing temperature so the influence of strain rate decreases.

Comparison with Experiments



- Lower modulus in experiments can be due to lower strain rates and the presence of defects in the experimental fibers.

Acknowledgements

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