Enhancing Polyethylene Fiber Strength: Insights from Molecular Dynamics

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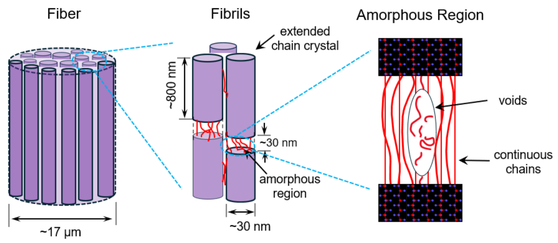
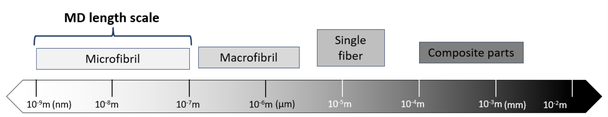
Introduction



- UHMWPE is widely used in numerous structural applications.
- Voids are commonly found between and inside fibrils that typically contains amorphous/unaligned chains.
- Understanding the effects of voids is essential for improving material properties.
- Molecular Dynamics (MD) simulations can be used to gain insight into the influence of voids on material properties.

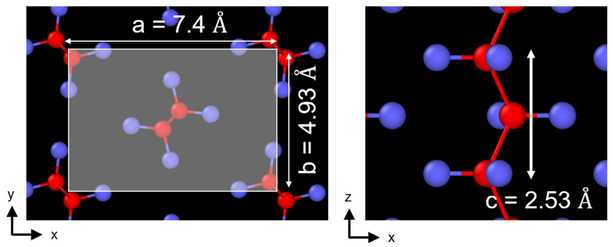
Method

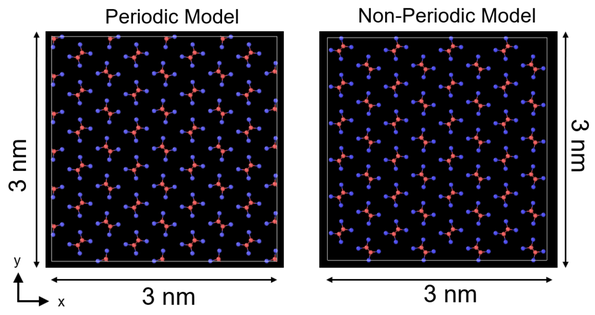
MD simulations of fibril containing amorphous and crystalline regions (with and without voids) → Multiscale finite element modeling of UHMWPE fibers



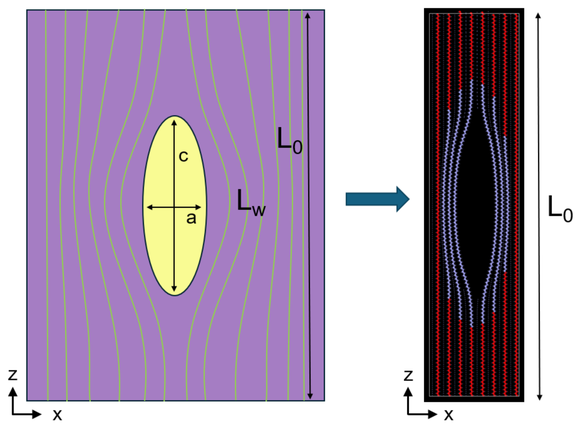
- Used LAMMPS with AIREBO-M potential to conduct MD simulations.
- Postprocessing was done in MATLAB and OVITO.
- A single PE chain consists of ~100 monomers (600 atoms). The model contains 56 chains.

UHMWPE Unit Cell





3D Void Model

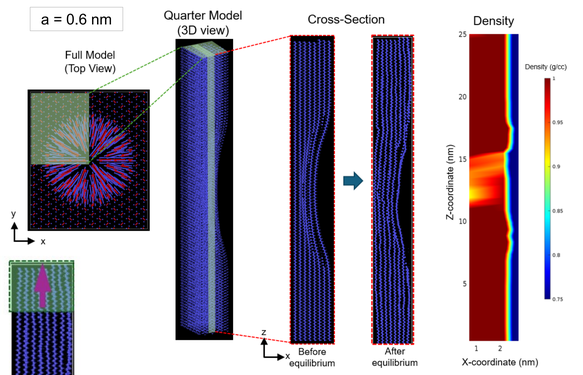


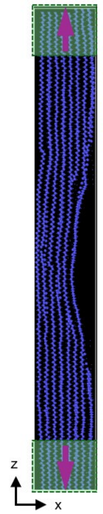
L_w is the length of the curved chains

Model	Pristine	a = 0.6 nm	a = 1.2 nm
L_w/L_0	1.00	1.05	1.07

- Higher length ratio corresponds with longer chains that withstand larger strains during progressive failure.

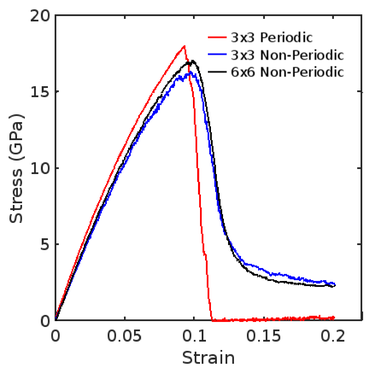
Quarter Void Model Creation





- Longer chains collapse to decrease density below crystalline density (1.01 g/cm^3).
- Length of the fixed ends is ~0.6 nm.
- Tensile tests were conducted at 300 K under a strain rate of 10^9 s^{-1}.
- Stress was computed by dividing the average end force by the cross section area near ends.

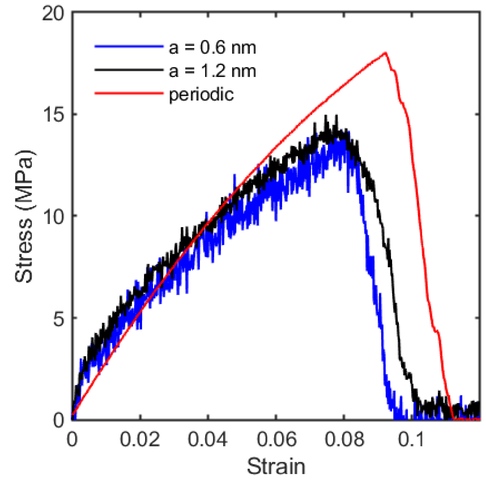
Effects of Free Surface



Model	3x3 Periodic	3x3 Non-Periodic	6x6 Non-Periodic
Strength (GPa)	18.0	16.3	17.1
Modulus (GPa)	263	226	243

- Stress-strain curves of non-periodic models approaches that of the periodic model as the model size increases.
- Large model Non-periodic model has higher residual stress due to chain sliding.

Effect of Voids



Model	Pristine	a = 0.6 nm	a = 1.2 nm
Strength (GPa)	18.1	14.3	14.9
Modulus (GPa)	263	323	359

- The curvature of the chains generate non-equilibrium bond lengths and angles, resulting in much stiffer bonds. This increases the effective stiffness of the middle region, (a topic for future study).
- Peak stress decreases in the presence of void due to progressive failure, i.e., straight chains fail first.

Acknowledgements

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