Micromechanical model of the plasticity and failure behavior of highly oriented polyethylene fibers

H. Dong, Z. Wang, A. Azoug, T. O’Connor, M. Robbins, and T. D. (Vicky) Nguyen*
Email: vicky.nguyen@jhu.edu

Background

- Constitutive Relations
  - Amorphous domain: Isotropic viscoplasticity (Gowndjee, 1998)
    - $E = 1.0 \text{ GPa, } v = 0.2, \tau_0 = 0.04 \text{ GPa}$
  - Crystal domains: Crystal plasticity model (Marin 2006)
    - Anisotropic elastic constants and slip strengths from MD simulations (O’Connor et al., 2015)

- Several studies have shown that UHMWPE fibers present a complex morphology composed of interlocking shish-kebab structures.
- Despite the degree of crystallinity of the fibers (>95%), the tensile modulus and strength remains below the theoretical value of UHMWPE crystals.

Key Goals

This work aims at determining the origin of this discrepancy by investigating the relations between the morphology and the mechanical properties.

Technical Approach

- Honeywell UHMWPE fibers
  - Crystallinity 85% (McDaniel et al., 2015)
  - Oriented crystal diameter $d_0 \approx 20 \text{ nm}$
  - Lamellar interweaving domain
    - Thickness $T_1 = 35 \text{ nm}$ (McDaniel et al., 2015)
    - Diameter $d_1$ - determined from % crystallinity and oriented domain size

- Varying lamellar connectivity to oriented domains

Transverse compression: effect of amorphous phase and morphology

- Young’s modulus and yield strength increase significantly for $E_{\text{amorph}} > 1 \text{ GPa}$ domain.
- Higher yield strength for more lamellar connections

Major Results

- Young’s modulus and yield strength increase significantly for $E_{\text{amorph}} > 1 \text{ GPa}$ domain.
- Higher yield strength for more lamellar connections

Future Directions in 2017

- Investigate the effect of cracks and voids on modulus and failure strength of the fibrils, including effect of the porosity and size distribution of voids and cracks
- Examine the effect of distribution in size of the crystalline domains and variations in their orientation

Impact

- Understanding the structural basis for the mechanical and failure properties is needed to design materials and processing methods that enhance stiffness, strength, and toughness properties of the fibers.
- The theoretical and computational models developed by the study will provide guidelines and computational design tools for armor and other structural applications of the oriented polymer fibers.