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Thermal and Mechanical Properties of Polymer Nanofibers from Molecular Simulations SEZEN CURGUL, KRYSTYN J. VAN VLIET, GREGORY C. RUTLEDGE, MIT — Polymer nanofibers exhibit new, emergent behavior as the diameter of the fibers are decreased from macroscopic to nanometer length scales. Since individual nanofibers are challenging to characterize experimentally due to their small size, computer simulations can be helpful in predicting the properties. We present the results of molecular dynamics (MD) simulations of polymer nanofibers to study their size-dependent properties. The fibers mimic the prototypical polymer polyethylene and have diameters in the range 2.0 to 23.0 nm. The fibers have been analyzed size dependent behavior in their thermal and mechanical properties. The glass transition temperature (Tg) of these amorphous nanofibers decreases with decreasing fiber diameter, and is independent of molecular weight over the range considered. Application of a volume averaged layer model for Tg shows that the cooperativity length scale compares well with previous estimates for polyethylene. Young's moduli of these nanofibers also decrease with decreasing fiber diameter, in agreement with T_g depression. There is a significant decrease in modulus when the temperature increases above the glass transition temperature of the surface layer.

Sezen Curgul
MIT

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