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Chain Ends and the Ultimate Tensile Strength of Polyethylene Fibers[1] THOMAS C. O'CONNOR, MARK O. ROBBINS, Johns Hopkins University — Determining the tensile yield mechanisms of oriented polymer fibers remains a challenging problem in polymer mechanics. By maximizing the alignment and crystallinity of polyethylene (PE) fibers, tensile strengths $\sigma \sim 6 - 7$GPa have been achieved. While impressive, first-principal calculations predict carbon backbone bonds would allow strengths four times higher ($\sigma \sim 20$GPa) before breaking. The reduction in strength is caused by crystal defects like chain ends, which allow fibers to yield by chain slip in addition to bond breaking.
We use large scale molecular dynamics (MD) simulations to determine the tensile yield mechanism of orthorhombic PE crystals with finite chains spanning $10^2 - 10^4$ carbons in length. The yield stress σ_y saturates for long chains at $\sim$ 6.3 GPa, agreeing well with experiments. Chains do not break but always yield by slip, after nucleation of 1D dislocations at chain ends. Dislocations are accurately described by a Frenkel-Kontorova model, parametrized by the mechanical properties of an ideal crystal. We compute a dislocation core size $\xi = 25.24$Å and determine the high and low strain rate limits of σ_y. Our results suggest characterizing such 1D dislocations is an efficient method for predicting fiber strength.

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