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To Slip or Snap: Finite Length Chains and Yield Mechanisms in Polyethylene Fibers[1] THOMAS O'CONNOR, MARK ROBBINS, Johns Hopkins University, Physics and Astronomy — Understanding the microscopic mechanisms of yield in oriented polymer fibers is a long -standing problem. Advances in polymer processing have produced highly ordered polyethylene (PE) fibers with tensile strengths between 4-7 GPa, but these values are far less than the theoretical limiting strength of 25 Gpa due to C-C bond scission. This reduction in strength is caused by the presence of defects within the fiber. The simplest type of defect is chain ends which reflect the finite length of polymer chains. The presence of chain ends allows a polymer fiber to yield by chain slip without scission of covalent bonds. Here we present extensive united atom (UA) and all atom (AA) molecular dynamics simulations of crystalline PE fibers subjected to uniaxial tension. The fibers are fully aligned crystals constructed from chains of finite length N, with N spanning 3 orders of magnitude ($10^1 - 10^4$ monomers). We explore the yield behavior of these systems and relate it to the dynamics of the underlying chain end defects. UA tensile strengths are systematically smaller than AA by a factor of about 3. Both show a saturation in tensile strength as N rises above 500 monomers. This reflects a saturation in the stress for chain ends to slip and implies a maximum tensile strength of 6 Gpa.

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