

Abstract Submitted  
for the MAR12 Meeting of  
The American Physical Society

**Molecular simulation of plastic deformation of semicrystalline polyethylene** JUNMO KIM, SANGHUN LEE, GREGORY RUTLEDGE, Massachusetts Institute of Technology — The detailed structure and the high anisotropy of semicrystalline polymer at the lamellar length scale play an important role in determining its mechanical response. In this study, we performed molecular dynamics simulation of semicrystalline polyethylene under various industrially important deformations, such as extension, compression, and shear, to characterize the plastic deformation response. The semicrystalline polyethylene model employed in this study consists of a 1-D alternating stack in the longitudinal z direction of crystalline lamellae and interlamellar noncrystalline domains, that are infinite in the lateral x and y directions. The molecular dynamics simulations are carried out at the temperature of 350K using united atom model and two deformation strain rates (fast and slow) are considered in each deformation. Stress-strain curves, elastic moduli, yield stresses and so on, are examined under each deformation and compared to each other. In addition, the entanglement statistics of semicrystalline polyethylene under various deformation modes are investigated using the Z-code.

Junmo Kim  
Massachusetts Institute of Technology

Date submitted: 11 Nov 2011

Electronic form version 1.4