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Plastic Deformation of Semicrystalline Polyethylene under Extension, Compression, and Shear using Molecular Dynamics Simulation JUN MO KIM, Massachusetts Institute of Technology, REBECCA LOCKER, ExxonMobil Research and Engineering Co., GREGORY RUTLEDGE, Massachusetts Institute of Technology — Molecular dynamics simulation has been performed to investigate the plastic deformation of semicrystalline polyethylene under various modes of deformation, such as extension, compression and shear. Many mechanical and structural properties of semicrystalline polyethylene are examined and compared with previous study [Lee and Rutledge, Macrmol. 44, 3096 (2011)]. Under tensile deformation, we observed crystallographic slip at low strains ($e_3 < 0.08$) regardless of deformation rate. However, two different yield mechanisms were monitored as a function of deformation rate at intermediate strains ($e_3 < 0.25$). At high strains ($e_3 > 0.25$), melting and recrystallization were observed for slow deformation ($5\times10^6 s^{-1}$) whereas cavitations were monitored for fast deformation ($5\times10^7 s^{-1}$). Under compressive deformation, stress-strain curve shows very similar behavior to tensile deformation at low strain, and crystallographic slip plays an important role for mechanical response of semicrystalline polyethylene. Under shear deformation, the chains tend to stretch and align into the shear direction. We also calculated stiffness constants for shear deformation and compared these to results of previous study [In't Veld et al. Macromol. 39, 439 (2006)]. Interestingly, semicyrstalline polyethylene shows typical transient behavior of Newtonian fluids under shear deformation, which we compare to various constitutive models, such as the Upper-Convected Maxwell (UCM) and Giesekus models.

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