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Molecular Dynamics Simulations of Homogeneous Crystallization in Polymer Melt BIN KONG, Chinese Academy of Sci (CAS) — Molecular mechanisms of homogeneous nucleation and crystal growth from the melt of polyethylene-like polymer were investigated by molecular dynamics simulations. The crystallinity was determined by using the site order parameter method (SOP), which described local order degree around an atom. Snapshots of the simulations showed evolution of the nucleation and the crystal growth through SOP images clearly. The isothermal crystallization kinetics was determined at different temperatures. The rate of crystallization, K_c, and the Avrami exponents, n, were determined as a function of temperature. The forming of nucleis was traced to reveal that the nucleis were formed with more ordered cores and less ordered shells. A detailed statistical analysis of the MD snapshots and trajectories suggested conformations of the polymer chains changed smoothly from random coil to chain folded lamella in the crystallization processes.

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