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Molecular simulations of the formation of semi-crystalline structure from supercooled polyethylene melt PENG YI, Johns Hopkins Univ — Formation of semi-crystalline structure is important for industrial processing, but it is scientifically poorly understood due to the strong anisotropy and the conformational flexibility of polymer chains. In this work we report the results of molecular dynamics simulations of homogeneous crystallization from polyethylene melts. A realistic united atom model was used. At room temperature (˜30% supercooling), the crystal nucleation and growth lead to a stable semi-crystalline structure, with crystal lamellae separated by amorphous regions. Entanglement in the amorphous region prevents further crystal growth. The crystal-amorphous interface migrates with changing annealing temperature. Chain segments in the amorphous region adopt loop, bridge and tail conformations. Their populations and lengths were calculated and analyzed.

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