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Molecular simulation of homogeneous crystal nucleation of n-alkane melts PENG YI, GREGORY RUTLEDGE, Massachusetts Institute of Technology — One of the most important phenomena in molecular systems is homogeneous nucleation of the crystal phase from a melt. This phenomenon is particularly interesting for chain molecules due to their strong anisotropy and their conformational flexibility. In this work we report the results of molecular simulations of homogeneous crystal nucleation of n-eicosane (C20) from the melt. A realistic united atom force field was employed. The crystal phase and melting behavior were first determined by ramping temperature in a set of MD simulations. The nucleation trajectory was then sampled using MD simulations at about 20% supercooling; and the nucleation free energy was sampled using Monte Carlo umbrella sampling method for three temperatures, ranging from 10% to 20% supercooling. A first-passage time technique was used to determine the critical nucleus and the nucleation rate. Detailed examination of the simulations reveals the critical nucleus to be a bundle of stretched segments about 8 CH2 groups long, organized into a cylindrical shape. The remaining CH2 groups form a disordered interfacial layer. By fitting the nucleation free energy curve to the cylindrical nucleus model, the crystal-melt interfacial free energies are calculated to be about 10 mJ/m2 for the side surface and 4 mJ/m2 for the end surface. We also discussed the effect of using different nucleus definitions

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