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Molecular simulation of crystal nucleation of n-alkane melts PENG YI, GREGORY RUTLEDGE, Massachusetts Institute of Technology — One of the most important phenomena in molecular systems is nucleation of the crystal phase from a homogeneous 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 crystal nucleation of n-alkane 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 molecular dynamics simulations. The adiabatic nucleation trajectory was then sampled using the molecular dynamics simulations and the Monte Carlo umbrella sampling method. A mean-first-passage-time technique was used to determine the critical nucleus and the nucleation rate. The cylindrical nucleus model was found to provide a better quantitative description of the critical nucleus than the spherical nucleus model. We were also able to calculate the interface free energy for the end and side surface of a cylinder nucleus model from the Monte Carlo simulation data without making further assumption. This method can be extended to study longer n-alkane molecules and the change of nucleus conformation as n increases.

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