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Molecular simulation of crystal nucleation of n-alkane melts PENG YI, GREGORY RUTLEDGE, Massachusetts Institute of Technology — The homogeneous nucleation of a crystal phase is one of the most interesting phenomena of molecular fluids, yet the microscopic mechanism of which still remains poorly understood. It is even more a mystery in chain molecule systems because the chain connectivity could produce very different crystal nucleus conformations, which are important factors in determining the subsequent crystal growth process and the properties of the final product. In this work we report the results of molecular simulations of crystal nucleation of n-alkanes 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 Monte Carlo umbrella sampling technique. The surface energy of the crystal nuclei was calculated assuming a spherical nucleus model and compared with previous studies to validate our numerical definition of a crystal nucleus. We were also able to calculate the end and side surface free energies of a cylinder nucleus model from the 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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