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Classical nucleation theory based method for computing the crystal-melt interfacial free energy XIAN-MING BAI, MO LI, School of Materials Science and Engineering, Georgia Institute of Technology — The crystal-melt interfacial free energy is a fundamental thermodynamic parameter governing phase transformations. It is very weak and extremely difficult to obtain experimentally. Here we present a simple approach, which is based on classical nucleation theory, for calculating the solid-liquid interfacial free energy. Using molecular-dynamics simulations, we construct spherical crystal nuclei embedded in the supercooled liquids to create an ideal model of homogeneous nucleation. The interfacial free energy is extracted by fitting the relation between the critical nucleus size and the reciprocal of the critical undercooling temperature. The orientationally averaged interfacial free energy is found to be 0.301 with errors of 0.002 (in standard LJ unit). The temperature dependence of interfacial free energy is also obtained in this work. We find that the interfacial free energy increases slightly with increasing temperature. The positive temperature coefficient of interfacial free energy is in good agreement with Spaepen's analysis [Solid State Phys. **47**, FS181, (1994)] and Turnbull's empirical estimation [J. Appl. Phys. **21**, 1022 (1950)].

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