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A New Method for Computing the Anisotropy in Crystal-melt Interfacial Free Energy. XIAN-MING BAI, MO LI, School of Materials Science and Engineering, Georgia Institute of Technology — The anisotropy in the crystal-melt interfacial free energy is very important for understanding the crystal growth morphology. In this work, we have performed molecular dynamics simulations to calculate the interfacial free energy and its anisotropy. By inserting crystal nuclei with different geometric shapes into a supercooled liquid, we determined the corresponding critical temperatures. The spherical, cubic, and bipyramidal nuclei were used in this work. Using the classical nucleation theory but with different geometric factors, we have calculated the interfacial free energies in different orientations.

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