Kinetic Coefficient for Hard-Sphere Crystal Growth from the Melt

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Abstract:

Using molecular-dynamics simulation, we determine the magnitude and anisotropy of the kinetic coefficient (μ) for the crystal growth from the melt for the hard-sphere system through an analysis of equilibrium capillary fluctuations in interfacial height. We find $\mu 100=1.44(7)$, $\mu 110=1.10(5)$, and $\mu 111=0.64(3)$ in units of $\sqrt{k_B/(mT_m)}$, where k_B is Boltzman's constant, m is the particle mass, and T_m is the melting temperature. These values are shown to be consistent, with some exceptions, with those obtained in recent simulation results a variety of fcc metals, when expressed in hard-sphere units. This suggests that the kinetic coefficient for fcc metals can be roughly estimated from $C\sqrt{R/(MT_m)}$, where R is the gas constant, M is the molar mass, and C is a constant that varies with interfacial orientation.