Crystal-melt interfacial free energy of binary hard spheres from capillary fluctuations

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Abstract:

Using molecular-dynamics simulation coupled with an analysis of equilibrium capillary fluctuations in interfacial position, we compute the magnitude and anisotropy of the interfacial free energy γ for a binary hard-sphere system with a diameter ratio $\alpha=0.9$. This system, in which the fluid mixture coexists with a randomly substituted face-centered-cubic solid solution, is a useful reference model for alloys. Our results show that γ increases with increasing mole fraction of the smaller sized particle when temperature is held constant. However, after rescaling the results to fixed pressure and varying temperature, we find that γ decreases with increased alloying by the smaller particle (corresponding to lower temperatures). Thus, γ is seen to decrease with increasing concentration of the lower melting point solute, consistent with earlier simulations on Ni/Cu and Lennard-Jones mixtures. The anisotropy in γ is such that the inequality $\gamma100>\gamma110>\gamma111$ holds for all concentrations studied. Using the classification scheme of Haxhimali et al., [Nat. Mater. 5, 660 (2006)] we find that the anisotropy in γ is consistent with a predicted $\langle 100 \rangle$ primary dendrite growth direction.