Calculation of the crystal-melt interfacial free energy for the binary hard sphere system with the diameter ratio of 0.9 at the zoetrope

Majeed Amini, Brian Laird (April 2011)

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Abstract:

Using the analysis of equilibrium capillary fluctuations in molecular dynamics simulations, we compute the magnitude and anisotropy of the interfacial free energy γ of the crystal-melt interface for the binary hard-sphere system with $\alpha = 0.9$ at the azeotrope. We found $\gamma100 = 0.62(2)$, $\gamma110 = 0.60(2)$, and

$\gamma111 = 0.58(2)$. We compare our results with the values of the interfacial free energy of the same system but at points other than azeotrope, as well as with the interfacial free energy of a single hard sphere system. Our results show the relation $\gamma100 > \gamma110 > \gamma111$ being consistent with the simulation results for

various metals, Lennard-Jones (LJ) system, and single hard-sphere system.