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Calculation of the crystal-melt interfacial free energy for the binary hard-sphere system with the diameter ratio of 0.9 at the azeotrope[1]
MAJEED AMINI, Department of Mathematical Science, Ahlia University, GUCCI Complex, Manama, Kingdom of Bahrain, BRIAN LARID, Department of Chemistry, University of Kansas, Lawrence, Kansas 66045, USA — Using the analysis of equilibrium cappillary 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 $\gamma_{100} = 0.62(2)$, $\gamma_{110} = 0.60(2)$, and $\gamma_{111} = 0.58(2)$. 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 $\gamma_{100} > \gamma_{110} > \gamma_{111}$ being consistent with the simulation results for various metals, Lennard-Jones (LJ) system, and single hard-sphere system.

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