

The kinetic coefficient of hard-sphere crystal-melt interfaces from molecular-dynamics simulations MAJEED AMINI, Department of Physics, University of Kansas, Lawrence, KS 66045 USA, BRIAN LAIRD, Department of Chemistry, University of Kansas, Lawrence, Kansas 66045 USA — The kinetic coefficient for a crystal melt interface, μ , is the ratio of the interface growth velocity to the undercooling ($T_M - T$), where T_M is the melting point. In this work we determine the kinetic coefficient for the hard-sphere system by analyzing capillary fluctuations in interface position using molecular dynamics (MD) simulation [Hoyt et al, Mat. Sci. Eng. R 41, 121-163 (2003)]. We report the kinetic coefficient for the three interfaces: (100), (110), and (111). Our results for μ_{100} , μ_{110} , and μ_{111} are $1.15(4) (k_B/(mT_M))^{1/2}$, $0.85(6) (k_B/(mT_M))^{1/2}$, and $0.57(8) (k_B/(mT_M))^{1/2}$, respectively, which gives the relation $\mu_{100} > \mu_{110} > \mu_{111}$. This ordering is consistent with the recent results of MD simulations for a variety of metals. The anisotropy ratios μ_{100}/μ_{110} , and μ_{100}/μ_{111} are $1.35(11)$, and $2.0(3)$, respectively. We compare our results to those of classical density functional theory (DFT) of [Mikheev and