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Ginzburg-Landau theory of the bcc-liquid interface kinetic coefficient KUO-AN WU, Department of Physics, National Tsing-Hua University, Hsinchu, Taiwan, JEFFREY HOYT, Department of Materials Science and Engineering and Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada, ALAIN KARMA, Physics Department and Center for Interdisciplinary Research on Complex Systems, Northeastern University, Boston, USA — We extend the Ginzburg-Landau (GL) theory of atomically rough bcc-liquid interfaces outside of equilibrium to derive an analytical expression for the kinetic coefficient $\mu(\hat{n})$. The kinetic coefficient is expressed as a spatial integral along the normal direction of a sum of gradient square terms corresponding to different nonlinear density wave profiles. Anisotropy arises naturally from the dependence of those profiles on the angles between the principal reciprocal lattice vectors $\vec{K}_i$ and $\hat{n}$. Values of the kinetic coefficient for the (100), (110) and (111) interfaces are compared quantitatively to the prediction of linear Mikheev-Chernov (MC) theory and previous MD simulation studies of crystallization kinetics for a classical model of Fe. The GL theory predicts a similar expression for μ as the MC theory but yields a better agreement with MD simulations for both its magnitude and anisotropy due to a fully nonlinear description of density wave profiles across the solid-liquid interface. In particular, the overall magnitude of μ predicted by GL theory is an order of magnitude larger than predicted by the MC theory. GL theory is also used to derive an inverse relation between μ and the solid-liquid interfacial free-energy.

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