Thermodynamic and Kinetic Properties of Solid-Liquid Interfaces from Atomistic Simulations

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It is well known that during the solidification of alloys, the shape and velocity of a growing dendrite depends critically on the anisotropy of the solid-liquid interfacial free energy, γ. We demonstrate that this anisotropy, although quite small, can be computed accurately from molecular dynamics simulations by monitoring the fluctuations in the height of the interface. Results are reported for Ag, Au, Cu, Ni and Pb where the embedded atom method is used to describe the interatomic potential. In addition, it will be shown how the interfacial stress, the excess energy and the excess entropy of the solid-liquid boundary can be obtained from atomistic simulations. In particular the excess entropy can be computed in two ways, from separate computations of both the excess energy and γ or from a direct calculation of the temperature dependence of the interfacial free energy. Results of the two methods will be compared and values of the excess quantities will be discussed in terms of existing models of the solid-liquid interface. Finally, the velocity of a planar interface as a function of undercooling has been computed for the low index directions [100], [110] and [111]. It will be shown that the velocity vs. undercooling results agree very well with a previously developed model of crystallization kinetics.