

Anisotropic Properties of Solid-Liquid Interfaces from Simulations

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Abstract:

This project is directed toward understanding crystal-melt interfaces, in particular the inherent anisotropy of interfacial energy and mobility. We have been testing and applying methods of calculating these properties at the atomistic level, through direct simulations of coexisting phases. These simulations are designed to complement ongoing experiments in the Solidification Sciences focus area.

Recent Results: We have performed molecular dynamics simulations of coexisting solid and liquid phases, such as the one shown at right. In this figure, the red atoms are disordered, in the liquid phase, while the blue and green atoms are ordered in the solid phase. The interface between the phases is rough, with the magnitude of the fluctuations determined by the interfacial stiffness, allowing for a measure of the stiffness and its anisotropy.

By measuring the fluctuations, we have calculated the complete anisotropic crystal-melt interfacial free energy of aluminum, finding an average free energy of $\sigma = 149 \text{ mJ/m}^2$ which is in reasonable agreement with current experimental results. The anisotropy in the (100) plane is found to be 0.9%, close to the value of 0.97% measured for Al-4%Cu measured by Shan Liu, Ralph Napolitano and Rohit Trivedi at Ames Lab.

Future Work: We are currently examining equilibrium fluctuations of the interface in Al to calculate the anisotropic interfacial mobility in this system. We are also calculating the anisotropic interfacial free energy for the Lennard-Jones and soft-sphere systems, to better understand the origin of anisotropy. We will eventually extend this work to binary systems.

Interactions: This work is being performed in close contact with other researchers involved in the Solidification Sciences focus area, in particular Ralph Napolitano, Rohit Trivedi and Shan Liu. A new collaboration with Xueyu Song (Dept. of Chemistry, Iowa State University) has been initiated this year. We are also participating in a Department of Energy sponsored “Computational Materials Science Network” on Microstructural Evolution based on Fundamental Interfacial Properties (Tony Rollett, David Srolovitz, and Alain Karma, Principal Investigators).

