Atomic-Scale Modeling of Solid-Liquid Interfaces and Phase-Equilibria in Alloys

M. Asta[1], J. J. Hoyt[2], A. van de Walle[1], V. Ozolins[3], M. van Schilfgaarde[3], and A. Karma[4]

[1] *Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60091, USA*

[2] *Sandia National Laboratories, Albuquerque, NM 87185, USA*

[3] *Sandia National Laboratories, Livermore, CA 94551, USA*

[4] *Department of Physics and CIRCS, Northeastern University, Boston, MA 02115, USA*

Molecular-dynamics and Monte-Carlo simulations are applied to the study of solid-liquid phase-equilibria and the equilibrium properties of solid-liquid interfaces in alloys. Computer simulations are based on the use of semi-empirical, many-body potentials and first-principles methods, including ab-initio molecular dynamics, to model interatomic interactions. We present results for liquid Al-Ni and Al-Cu alloys, discussing the origin of the highly non-ideal solution-thermodynamic properties in these systems. For Al-Cu we present results for the equilibrium structural and thermodynamic properties of solid-liquid interfaces as a function of crystallographic orientation. The link between these atomic-scale calculations of solid-liquid interface properties and phase-field models of solidification-microstructure evolution will be discussed.