# Determining the Structure, Thermodynamics and Kinetics of Solid-Liquid Interfaces and Grain Boundaries by Computer Simulation

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The thermodynamics and growth kinetics of interfaces in condensed matter systems are largely controlled primarily by two quantities: the interfacial free energy and the kinetic coefficient. The interfacial free energy between two coexisting phases, γ, is the amount of work required to reversibly form a unit area of interface. The kinetic coefficient, μ, is the constant of proportionality between the growth velocity of an advancing interface and the undercooling, ΔT. Accurate values of both γ and μ are necessary for the full understanding of a number of technologically important phenomena in chemistry and materials science, such as dendritic crystal growth, crystal nucleation, wetting, liquid-metal embrittlement, and others. However, reliable experimental results are challenging and rare, so atomistic simulation remains an important means of determining the thermodynamic phenomenology of such systems. The previous work of in the Laird Group1-3 and others on model and realistic systems has established computer simulation as useful technique for the understanding of the generic and specific phenomenology of crystal-melt interfaces. Specific subprojects that are possibilities for an REU research project are

- Further development and evaluation of a new method, based on Cahn's extension of Gibbs' interface thermodynamics, to quantify the dependence of γ on atomic and molecular interactions
- Development and application of direct methods (cleaving and lattice switch) to calculate grain-boundary free energies
- Adaptation of existing methods from our group to the interface thermodynamics and structure of chemically heterogeneous solid-liquid interfaces
- Adaptation of existing methods to the calculation of γ for molecular systems, including binary mixtures
- Adaption of cleaving method to calculate γ for solid-liquid interfaces with long range interactions, for example, ionic salts and colloids

[1] P. Palafox-Hernandez, B.B. Laird and M. Asta, "Atomistic characterization of the Cu-Pb solid-liquid interface", Acta. Mater. 59, 3137¬–3144 (2010).

[2]B.B. Laird and R.L. Davidchack, "Calculation of the interfacial free energy of a fluid at a static wall by Gibbs-Cahn integration", J. Chem. Phys, 132, 204101 (2010).

[3]B.B. Laird, R.L. Davidchack,Y. Yang and M. Asta, "Determination of the solid-liquid interfacial free energy along a coexistence line by Gibbs-Cahn integration", J. Chem. Phys. 131, 114110 (6 pages) (2009).