Atomistic Modeling of Tin Surface and Grain Boundary Diffusion

Michael S. Sellers[1]*, Andrew J. Schultz[1], Cemal Basaran[2], and David A. Kofke[1]
[1]*Department of Chemical and Biological Engineering*
[2]*Electronics Packaging Laboratory,*
Department of Civil, Structural and Environmental Engineering
University at Buffalo, The State University of New York, Buffalo, NY 14260

The field of nanoelectronics packaging can benefit from the analysis and understanding of atomic level failure processes in thin films and lead-free solder joints. Imperfections in these interconnects—surfaces and grain boundaries in tin—provide fast diffusion paths for solute atoms, alloyed compounds, and atomic vacancies. In addition, all are given a strong diffusive force resulting from the high amount of electric current flowing through the joints. Modeling these specific diffusive processes and quantifying the diffusivity of tin atoms and vacancies will aid in the prediction of damage rates for these types of joints—key parameters for the realization of nanoelectronics.

Two methods of molecular simulation are used to compute the diffusivity of tin atoms in our systems. First, common molecular dynamics simulations are used to determine an overall atomic diffusivity in varying angles of symmetric tilt grain boundaries. Second, we use a potential energy surface walking method, called the Dimer method, to seek out diffusion mechanism saddle points in a molecular statics style simulation. From the Dimer method results, we can use harmonic transition state theory to compute tracer diffusivities of tin in our surface and grain boundary systems. These methods are compared and quantitative values for activation energies and diffusion coefficients are presented.

*Poster presenting author.