Molecular Simulation of

# Atomistic Transport and Microstructure of Tin-Silver-Copper Solder

## BACKGROUND

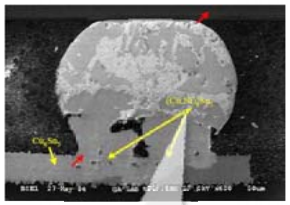
### Solder joints

in *nanoelectronics* will feel a high electrical current density from a decrease in cross-sectional area

### Increased damage

results from high *current density* and a large temperature gradient

Electromigration and Thermomigration →



### Microstructure

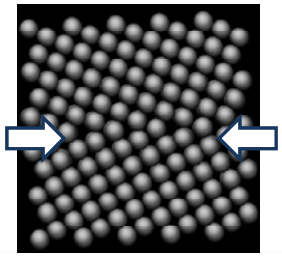
of the solder joint controls its strength and rate of damage

Orientation colored polycrystalline tin →

### Grain boundaries

provide fast diffusion paths for vacancies and solute atoms

Disordered interface created by two grains →



## WHAT CAN WE GET FROM MOLECULAR SIMULATION?

### Quantitative Predictions of Material Properties

Using well developed interatomic potentials to represent the components of lead-free solder, we can compute accurate material properties of the tin-silver-copper system.

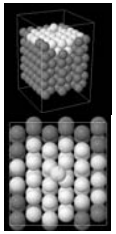
### An Understanding of Atomic Level Processes

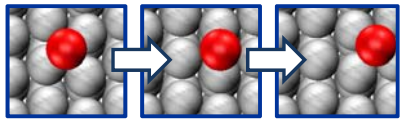
With simulation we get a view of the nanoscale. Molecular dynamics simulations allow us to visualize the structural processes that occur on the order of picoseconds, resulting from macroscale driving forces.

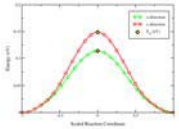
## RESULTS FROM MOLECULAR STATICS & DYNAMICS SIMULATIONS

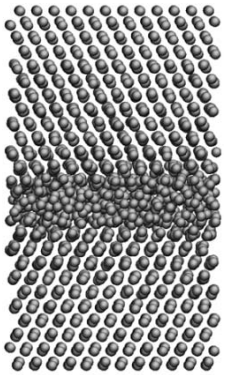
### Tin Surface Energies and Diffusion Coefficients

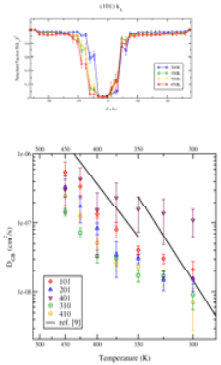
We calculate the surface energies of various Miller planes of tin and compute diffusivity on the (101) surface using the Dimer method.











### Tin Grain Boundary Structure and Diffusion Coefficients

Using molecular dynamics, we compute the grain boundary diffusivity of tin and analyze its structural response due to temperature and various types of grain boundaries.

EPL
Buffalo

NRL
Tabuk