Copper Diffusion in Silicon
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Copper is one of the major impurities found in silicon, and is known to induce a variety of adverse effects on the capabilities and reliability of silicon devices. Of particular interest, both scientifically and technologically, is the combination of extraordinarily high diffusivity and low solubility at room temperature. These properties have not only led to experimental difficulties in fully characterizing the physics and chemistry of copper in silicon, but make copper an especially difficult contaminant to remove from semiconductor devices.

Simulation cell: 512 Si atoms, 1 Cu atom for 5 nanoseconds of NVE dynamics.

We have used results from DFT calculations to fit the ReaxFF parameters and create a ReaxFF description of copper in the silicon lattice. We have used this ReaxFF description to simulate diffusion and compute diffusion coefficients for copper in silicon at three different temperatures (600K, 900K and 1200K). Our diffusion coefficients are in good agreement with experimentally observed values at the specified temperatures. We are now using ReaxFF to describe more complex aspects of the effects of copper impurities in silicon—such as inter-diffusion and precipitation.