Strain Effects on Thermal Transport in 2-D Nanocomposites

Yaoyao Xu and Gang Li
Department of Mechanical Engineering
Clemson University
Clemson, SC 29634

A recent area of research is about reducing the effective thermal conductivity of thermoelectric materials by using nanocomposites. While many encouraging results on the thermal transport in nanocomposites have been obtained from computational analysis, another important factor, namely the strain effect, has not been studied in the context of nanoscale thermoelectric composite materials. It is known that externally induced strain will cause a significant change in the phonon density of states, mean free path and relaxation time, which will in turn alter the thermal transport properties of nanocomposites. The study of the strain effects on the thermal transport could add another dimension to the design space of thermoelectric nanocomposites.

In this work, we investigate the strain effects on the thermal transport properties of 2-D nanocomposites. We focus on the calculation of the thermal conductivity of a Si/Ge composite with silicon wires embedded in germanium host and a layered Si/Ge structure, under various strain conditions. In the nanoscale, due to the ballistic phonon transport, the classical heat conduction theory is not valid. It has been shown that the thermal transport in nanocomposites can be more accurately described by the phonon Boltzmann equation. In this study, we incorporate the strain effects into the phonon Boltzmann equation through the strain dependent group velocity and phonon mean free path. The diffuse mismatch model is employed to calculate the interface phonon scattering between the silicon and germanium components. By solving the phonon Boltzmann equation we compute the phonon intensity in the nanocomposites. Once the phonon intensity is obtained, the effective temperature distribution can be calculated straightforwardly. The heat fluxes are computed by integrating the phonon intensity over the whole solid angle. The effective thermal conductivity is then calculated by using Fourier's law.