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Phonon Thermal Transport in SiGe-based Nanocomposites for Thermoelectric Applications ZLATAN AKSAMIJA, University of Massachusetts-Amherst — Silicon-germanium (SiGe) and $Si/Si_{1-x}Ge_x$ superlattices (SLs) have been proposed for application as efficient thermoelectrics because of their low thermal conductivity, below that of bulk $Si_{1-x}Ge_x$ alloys. However, the cost of growing SLs is prohibitive, so nanocomposites, made by a ball-milling and sintering, have been proposed as a cost-effective replacement with similar properties. Lattice thermal conductivity in SiGe SLs is reduced by scattering from the rough interfaces between layers. Therefore, it is expected that interface properties, such as roughness, orientation, and composition, will play a significant role in thermal transport in nanocomposites and offer many additional degrees of freedom to control the thermal conductivity in nanocompoosites by tailoring grain size, shape, and crystal angle distributions. We previously demonstrated the sensitivity of the lattice thermal conductivity in SLs to the interface properties, based on solving the phonon Boltzmann transport equation under the relaxation time approximation. Here we adapt the model to a broad range of SiGe nanocomposites. We model nanocomposite structures using a Voronoi tessellation to mimic the grains and their distribution in the nanocomposite and show excellent agreement with experimentally observed structures. In order to accurately treat phonon scattering from a series of atomically rough interfaces between the grains in the nanocomposite, we employ a *momentum-dependent* specularity parameter $p(\mathbf{q})=\exp(-4\pi^2\Delta^2 q^2\cos^2\theta)$. Our results show highly anisotropic thermal transport in SiGe nanocomposites below their bulk alloy counterparts.

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