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# A Monte-Carlo study of the phonon transport in nanowire-embedded composites

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ABSTRACT

This work aims at investigating the thermal conductivities of nanowire-embedded composites in use of a Monte-Carlo simulator developed based on the assumptions of grey media, bulk phonon dispersion relations, and bulk intrinsic scattering rates. Those along and those perpendicular to the wire axis direction are both targeted. The simulation results show that when the interface surfaces are totally diffuse, the cross-wire thermal conductivities of either the silicon-wire-germanium-host or germanium-wire-silicon-host nanocomposites decrease with increasing wire volume fraction due to the increasing, dominant, interface scattering; when the interface surfaces are perfectly smooth, a competition exists between the decreasing intrinsic and increasing interface scatterings as the wire volume fraction increases and a minimum thermal conductivity associated with the silicon-wire-germanium-host composite is existent. When heat flows mainly along the wire axis direction in either the wire-host composites or the double-layered nanowires, the interface and boundary effects dominate the effective thermal conductivities of the two components, which together with the cross-sectional-area ratio determine the major heat pathway. A minimum effective thermal conductivity can thus also be observed when these two factors are well-matched in strength and when the effective thermal conductivity of the nanowires is larger than that of the host/shell component.



## 1. Introduction

It is well known that the figure-of-merit $Z = S^2\sigma/k$ determines the efficiency of thermoelectric materials, where $S$, $\sigma$, and $k$ are the Seebeck coefficient, electric conductivity, and thermal conductivity respectively. Recent investigations have shown that the power factor $S^2\sigma$ can be enhanced by employing low-dimensional structures [1–4] and the thermal conductivity can be reduced by introducing heterogeneous interfaces or grain boundaries [5–7]. Among all, composites with properly designed internal nanoscaled structures have a higher ratio of the interface surface to the total volume, resulting in strong and frequent interface scatterings and thus a significant thermal-conductivity reduction. A thermal conductivity even lower than the bulk alloy counterpart becomes possible. An optimized nanostructure and optimized geometric parameters for given materials however have not been obtained. It is too expensive to find the answer experimentally and too intractable to solve it analytically. Numerical simulations are seemingly the best way to do. In this work, we aim at exploring the thermal-conductivity reduction associated with nanowire composites composed of silicon and germanium and finding any possible optimization of the relevant geometric parameters in use of the Monte-Carlo simulator.

The Monte-Carlo method is one of the numerical methods used to solve the Phonon Boltzmann transport equation (PBTE). In this method, the phonon distribution is discretized in the space as well as in the frequency domain. Phonon bundles then drift at their group velocities and are scattered by various mechanisms. In the pioneer work of Peterson [8], a constant mean free path was assumed and the boundary cells were maintained at constant temperatures by updating the local phonon properties every time step in order to generate a heat flux in the system. Mazumder and Majumdar [9] proposed a scattering probability as a function of the frequency and temperature, lumped the N and U processes into a single relaxation time, and treated the scattering by impurities in isolation. A genetic algorithm was carefully designed by Chen et al. [10], in which both the momentum and the energy are conserved during N processes and only energy is conserved during U processes. Moreover, the constant-temperature boundary condition was maintained by injecting phonons carrying properties at the prescribed temperatures from the boundaries. Lacroix et al. [11] suggested a new distribution function accounting for the collision processes. Phonons' directions are not changed if they suffer an N process to approximately preserve momentum. Randrianalisoa and Baillis [12] proposed a single-particle steady-state Monte-Carlo simulation scheme. The scheme is less memory demanding but

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