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Research Paper

Monte Carlo study of temperature-dependent non-diffusive thermal transport in Si nanowires

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HIGHLIGHTS

- The boundary scattering and length is investigated in thin silicon nanowires.
- Phonon Boltzmann transport equation is solved across a range of temperatures.
- Nanowire length plays an important role in silicon nanowires.

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ABSTRACT

Non-diffusive thermal transport has gained extensive research interest recently due to its important implications on fundamental understanding of material's phonon mean free path distributions and many nanoscale energy applications. In this work, we systematically investigate the role of boundary scattering and nanowire length on the non-diffusive thermal transport in thin silicon nanowires by rigorously solving the phonon Boltzmann transport equation (BTE) using a variance reduced Monte Carlo technique across a range of temperatures. The simulations use the complete phonon dispersion and spectral lifetime data obtained from first-principle density function theory calculations as input without any adjustable parameters. Our BTE simulation results show that the nanowire length plays an important role in determining the thermal conductivity of silicon nanowires. In addition, our simulation results suggest significant phonon confinement effect for the previously measured silicon nanowires. These findings are important for a comprehensive understanding of microscopic non-diffusive thermal transport in silicon nanowires.

1. Introduction

Nanowires, due to their unique electrical, thermal, and optical properties, have been a topic of extensive research interest for the past two decades [1–3]. Like other low-dimensional material structures [4,5], nanowires are promising for many practical applications, including, but not limited to, thermal management in nanoelectronic and optoelectronic devices [6–8], thermal interface materials [9,10], and thermoelectric energy conversion [11–14]. In particular, thermal transport in silicon nanowires (SNWs) have been extensively studied both experimentally and theoretically. For example, Volz and Chen computed the SNW thermal conductivity using molecular dynamics (MD) simulations and found nearly two orders of magnitude reduction in thin SNW thermal conductivity at room temperature [1]. In 2003, Li et al. [15] first experimentally measured the thermal conductivity of single-crystalline thin SNWs and observed substantial reduction in the measured thermal conductivity across a wide range of temperatures. They attributed the thermal conductivity reduction to increased phonon boundary scattering at the lateral walls of the nanowires and possible phonon confinement effect that may alter the bulk phonon dispersion relation. Two subsequent experimental studies [11,12] observed more than two orders of magnitude thermal conductivity reduction in their respectively synthesized on rough SNWs and SNW array with almost unaltered electrical conductivity and Seebeck coefficient, making them promising for high-performance and scalable thermoelectric materials.

On the other hand, various theoretical and numerical studies typically invoked MD simulations [16–19] and phonon Boltzmann

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transport equation (BTE) [2,20] to examine the role of boundary scattering, phonon confinement [21], phonon-surface-roughness scattering [22], and isotope scattering [16] on the thermal transport in SNWs. In particular, Chen et al. [20] used Monte Carlo simulations to investigate the effect of boundary scattering and phonon confinement on the thermal conductivity of thin SNWs. Yang et al. [16] observed exponential reduction in SNW thermal conductivity by isotopic defects at room temperature. Martin et al. [23] studied the effect of surface roughness on the thermal conductivity of SNWs and found a quadratic dependence of the thermal conductivity on the ratio of diameter to surface roughness for sub-100 nm sized nanowires. These simulation studies have helped gain insight into the nature of microscopic thermal transport in SNWs. However, these theoretical efforts typically neglect the impact of finite nanowire length on the nanowire thermal conductivity. Size effects can also occur when the nanowire length becomes comparable with the phonon mean free paths (MFPs). Non-diffusive thermal transport caused by finite nanowire length was only recently reported from experimental measurements on SiGe NWs with variable lengths [24]. In particular, Hsiao et al. [24] observed that ballistic thermal transport in micro-fabricated SiGe nanowires can persist over ~8.3 μm, much longer than previously believed.

Although non-diffusive thermal transport in NWs plays an important role in many applications as the diameter and length of the nanowires incorporated in devices both become comparable with the heat-carrying phonon MFPs [25–31], to the best of our knowledge, few studies have devoted to a comprehensive theoretical and numerical understanding of non-diffusive thermal transport caused by both lengthscales simultaneously in such nanostructures. In this work, we systematically investigate the role of phonon boundary scattering and finite nanowire length on the non-diffusive thermal transport in SNWs. A common practice to measure the degree of non-diffusive thermal transport is the use of effective thermal conductivity for the given nanostructure. We calculate the effective thermal conductivity for SNWs of variable diameters, lengths, and boundary specularities across a range of temperatures by rigorously solving the full phonon BTE under the relaxation time approximation. The numerous simulations in this study use a recently developed variance reduced Monte Carlo technique to achieve high calculation accuracy and acceptable computational cost. The complete phonon dispersion and lifetime data calculated from first-principle density functional theory are used as inputs in the simulations without any adjustable parameters. We find that both the nanowire diameter and length play an important role in determining the thermal conductivity and interpretation for nanowire thermal conductivity must take into account the nanowire length when it becomes comparable with phonon MFPs. Our simulation results also suggest significant phonon confinement effect in the previously experimentally studied SNWs.

2. Simulation details

To gain insight into how different lengthscales affect the thermal transport in thin NWs, the full spectral phonon BTE must be solved [32]. Since it is computationally expensive to solve the BTE using a deterministic approach [33,34], we resort to a recently developed deviational MC technique to rigorously solve the multi-dimensional phonon BTE to study the thermal transport physics in square SNWs [35–37]. Under the relaxation time approximation, the deviational spectral energy-based phonon BTE in its general form is given by [32]:

$$\frac{\partial e_\omega}{\partial t} + \vec{V}_\omega \cdot \nabla e_\omega = -\frac{e_\omega - e_{\omega 0}}{\tau_\omega} \quad (1)$$

where ω is the phonon angular frequency, V_ω is the frequency-dependent phonon group velocity, τ_ω is the spectral phonon relaxation time, $e_\omega = \hbar\omega(f_\omega - f_\omega^{eq})$ represents the deviational phonon energy distribution that is the product of the phonon energy $\hbar\omega$ and the deviational phonon distribution $(f_\omega - f_\omega^{eq})$, and $e_{\omega 0}$ represents the local equivalent equilibrium deviational energy distribution function. The deviational phonon distribution $(f_\omega - f_\omega^{eq})$ is the difference between the local phonon distribution function f_ω and the Bose-Einstein distribution function $f_\omega^{eq} = \frac{1}{\exp\left(\frac{\hbar\omega}{k_B T_{eq}}\right)+1}$ evaluated at a reference temperature T_{eq}. The advantage of solving the deviational energy-based phonon BTE instead of the original form is two-fold [35,36]. On one hand, it allows the energy conservation to be conserved automatically by conserving the number of computational phonon particles in the simulation domain. One the other hand, it allows simulations with high accuracy to be accomplished since we only simulate the deviation from a known reference equilibrium distribution that has analytical transport solution and therefore does not cause any stochastic noise in the final solution.

Details of the MC algorithm has been extensively described elsewhere [35,36,38–40] and are discussed briefly here. In this work, we study the thermal conductivity of SNWs across a set of temperatures where relaxation time approximation is applicable for silicon. For each temperature, a temperature difference $\Delta T = T_h - T_c = 1$ K is imposed on the two ends of the SNW, where T_h is the hot end temperature and T_c is the cold end temperature. By taking the reference temperature to be T_c, computational phonon particles are emitted only from the hot end of the NW (i.e. no phonons are emitted from the cold boundary since the deviational energy is exactly zero at the cold side) and they subsequently travel inside the NW subject to anharmonic scattering and boundary scattering. Phonon boundary scattering occurs if one computational particle encounters the lateral boundary of the nanowire during one specific advection step. In the occurrence of boundary scattering, resetting the phonon traveling direction depends upon the boundary specularity. Normally, a random number is drawn and compared to the boundary specularity. If the random number is smaller than the specularity, phonons are specularly reflected at the boundary; otherwise, it is diffusely scattered and its traveling direction is randomized into the simulation domain. Phonon-phonon scattering occurs if the particle does not collide with the boundaries in one advection step. All the phonon states, including frequency, group velocity, branch, and traveling direction, are reset in the event of phonon-phonon scattering. Since the temperature difference is small across the entire simulation domain, the scattering term in the phonon BTE can be linearized (as explained in Ref. [34]), resulting a significant simplification and efficiency gain because the computational particles can be simulated sequentially. The simulation of one particle ends when it is absorbed by either the hot end or the cold end. By looping the particles, we sample the contribution from all the simulated particles to find the heat flux and local temperature. The effective thermal conductivity of the NW is calculated through: $k_{eff} = Q/A\Delta T$, where Q is the heat flux across the NW and A is the cross-sectional area, respectively. In the limit of long nanowire, size effect results merely from the phonon boundary scattering. However, when the wire length becomes comparable with the phonon MFP, both the wire diameter and length affect the thermal transport [41].

3. Results and discussion

The developed simulation framework is applied to single-crystalline silicon nanowires of variable diameters and lengths to study the non-diffusive thermal transport behavior across a range