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Thermal conductance of cylindrical semiconductor nanowires modulated with phonon cavity

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A B S T R A C T

We study the effects of phonon cavities on the thermal conductance of cylindrical semiconductor nanowires by applying the scatter matrix method in combination with elastic wave continuum model. Our results show that the phonon cavity can enhance thermal conductance because of model coupling between phonon modes aroused in the phonon cavity, and phonon modes in the constrictions at lower temperatures. As the length of the phonon cavity increases, an oscillatory decay of the thermal conductance is exhibited at high temperatures. Compared with phonon cavities with lower wave velocities, phonon cavities with a higher wave velocity featured reduced thermal conductance at high temperatures. A brief analysis of these results is given.

1. Introduction

Recently, the thermal transport properties of nanostructures associated with phonons have attracted considerable attention both theoretically [1–9] and experimentally [10–12] for their potential applications to field-effect transistors [13], miniaturized optoelectronic devices [14], phonon devices [15], and heating cables [16]. When devices are scaled to the nanoscale, thermal dissipation becomes an important issue in nanoelectronics devices consisting of high density parts. Some studies have indicated that the limitations on thermal dissipation mainly arise from the interface of the nanostructure [17,18]. In addition, it has been proposed that the thermoelectric properties of nanostructures can be enhanced through structural design [19,20]. Hence, quantitative studies of the thermal transport of nanostructures is of great importance for preserving their desired functionalities in applications to thermal management and thermoelectrics. Phonon thermal properties have been reported for various kinds of nanostructures, including nanowires [21,22], nanoribbons [23,24], and nanotubes [25,26]. Furthermore, several intriguing physical effects including nonlinear thermal transport [27,28], thermal rectification [29,30], and negative differential thermal resistance [31,32] have been found. Previous studies have shown that discontinuities of the structure efficiently reduce thermal conductance by reducing phonon transmission. Such discontinuities include abrupt junctions [33], rough surfaces [34], and structural defects [35]. However, in some special situations, discontinuities in the structure can enhance the thermal conductance of semiconductor nanostructures. For instance, Huang et al. [36] reported that the low thermal conductance of two-dimensional rectangular semiconductor nanowires can be enhanced with a phonon cavity. Their work only focused on the effects of phonon cavity width on the thermal conductance in a two-dimensional rectangular nanowire at low temperatures. The effects of the elastic constants and geometric parameters of the wires and the cavity on the thermal conductance were not considered. Furthermore, ballistic thermal transport properties of cylindrical semiconductor nanowires have more practical significance than the thermal transport properties of rectangular nanowires. Chang et al. [37] reported on the frequency-dependent acoustic phonon transport through a cylindrical nanowire-bulk contact; however, their findings were restricted to the frequency conditions.

In this paper, using the scatter matrix method in combination with the elastic wave continuum model, we investigate the thermal transport properties of cylindrical semiconductor nanowires modulated with a phonon cavity. We study the effects of the wave velocity and geometric parameters of the phonon cavity on the ballistic thermal conductance properties in cylindrical semiconductor nanowires. Our results show that the phonon cavity can en-

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hance the thermal conductance at very low temperatures owing to the model coupling between phonon modes aroused in the phonon cavity and phonon modes in the constrictions. However, at high temperatures, the phonon cavity can reduce the thermal conductance because of phonon scattering by the discontinuous interfaces of the phonon cavity. The phonon transport coefficient is analyzed to better understand this interesting phenomenon. The influence of the wave velocity and geometry size of the phonon cavity on thermal transport also is considered. We find that a phonon cavity with a greater wave velocity can reduce the thermal conductance at high temperatures. As the length of the phonon cavity increases, oscillatory decay of the thermal conductance is exhibited at high temperatures. Our results suggest that the thermal conductance of cylindrical semiconductor nanowires can be modulated by the phonon cavity.

The paper is organized as follows. In Section 2, we give a brief description of the model and the necessary formulate used in the calculations. In Section 3, we compare the effects of various type nanowires, having different materials and various phonon cavities with different wave velocities, on the thermal conductance. Finally, we summarize our results in Section 4.

2. Computational details

In the present work, by applying the scatter matrix method in combination with the elastic wave continuum model, we investigate the thermal transport properties of a phonon cavity (region III) connecting two constriction regions (region II/region IV) between two semi-infinite cylindrical semiconductor nanowires, as shown in Fig. 1. For the model considered here, the expression of the thermal conductance K in the ballistic region can be written as [38]:

$$K = \frac{\hbar^2}{K_B T^2} \sum_m \frac{1}{2\pi} \int_{\omega_m}^{\infty} \tau_m(\omega) \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2} d\omega, \quad (1)$$

where $\hbar$, k_B, T, and ω_m are the reduced Planck's constant, Boltzmann constant, temperature and the cut-off frequency of the m-th mode, $\beta = 1/(k_B T)$, respectively, and $\tau_m(\omega)$ is the transmission coefficient of the m-th mode at frequency ω from region I across all the interfaces into region V. The transmission coefficient $\tau_m(\omega)$ can be effectively calculated by the scattering matrix method. For further details of the scattering matrix method, see Li et al. [38].

At low temperatures, based on the theory of elastic continuous model, the phonon displacement $U(r, \theta, z)$ in the cylindrical coordinate satisfies the following equation:

$$\upsilon^2 \nabla^2 U + \omega^2 U = 0, \quad (2)$$

where $\upsilon = \sqrt{C_{44}/\rho}$ is the wave velocity related to the mass density ρ and elastic stiffness constant C_{44}, and ω is the vibrational frequency of the phonon. The values of elastic stiffness constant and mass density for the considered materials are $C_{44}(\text{Si}) = 7.96 \times 10^{10}$ N/m^2, $C_{44}(\text{GaAs}) = 5.99 \times 10^{10}$ N/m^2, $C_{44}(\text{AlAs}) = 5.69 \times 10^{10}$ N/m^2, $\rho(\text{Si}) = 2300$ kg/m^3, $\rho(\text{GaAs}) = 5317$ kg/m^3 and $\rho(\text{AlAs}) = 3760$ kg/m^3 [39].

3. Results and discussion

Fig. 2 describes the calculated total thermal conductance K as a function of the temperature T for all five systems. Fig. 2(a) and 2(b) correspond to the system M1–M2 and M3–M5, respectively. Fig. 2(a) shows that as $T \to 0$ the conductance values of both M1 and M2 approaches their ideal value. As the temperature T increases, the thermal conductance of both M1 and M2 first decreases from the ideal value and then increases monotonously. The

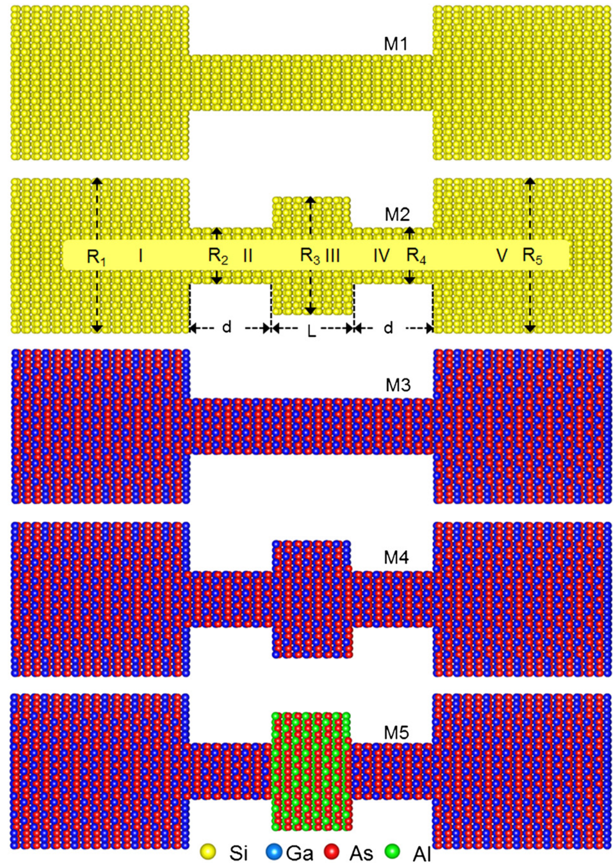

Fig. 1. Structures of the cylindrical semiconductor nanowires with a phonon cavity. Region III affects the properties of the phonon cavity when $R_3 > R_2$, where M1 and M3 correspond to Si and GaAs nanowires with $R_1 = R_5$, $R_2 = R_3 = R_4$, and $R_1 > R_2$, M2 and M4 correspond to Si and GaAs nanowires with $R_1 = R_5$, $R_2 = R_4$, and $R_3 > R_4$, and M5 corresponds to an GaAs nanowire where region III is replaced by AlAs.

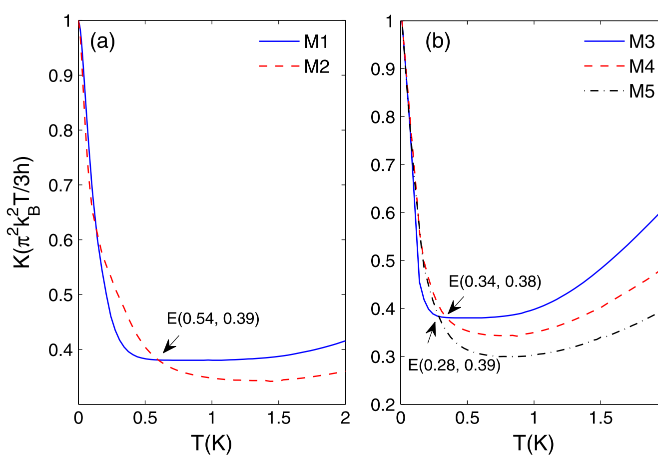

Fig. 2. Total thermal conductance K as a function of the temperature T for M1–M5. Here, we take $R_1 = R_5 = 30$ nm, $R_2 = R_4 = 20$ nm, $d = 20$ nm, and $L = 50$ nm. For M1 and M3, $R_3 = 20$ nm. For M2, M4, and M5, $R_3 = 25$ nm.

transformation of the thermal conductance can be attributed to the intrinsic transport of the phonon mode. Taking M1 as an example: at low temperatures ($T < 0.54$ K), only the zero-phonon mode can be aroused and is scattered by the discontinuous interfaces in the transmission process. At high temperatures ($T > 0.54$ K), the high index phonon mode is gradually excited and can contribute to the thermal conductance. Thus, the thermal conductance for all five systems first decreases from the ideal value and then