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Thermal conductance associated with six types of vibration modes in quantum wire modulated with quantum dot

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ABSTRACT

We study the ballistic phonon transport and thermal conductance of six low-lying vibration modes in quantum wire modulated with quantum dot at low temperatures. A comparative analysis is made among the six vibrational modes. The results show that the transmission rates of the six vibrational modes relative to reduced frequency display periodic or quasi-periodic oscillatory behavior. Among the four acoustic modes, the thermal conductance contributed by the torsional mode is the smallest, and the thermal conductances of other acoustic modes have adjacent values. It is also found that the thermal conductance of the optical mode increases from zero monotonously. Moreover, the total thermal conductance in concavity-shaped quantum structure is lower than that in convexity-shaped quantum structure. These thermal conductance values can be adjusted by changing the structural parameters of the quantum dot.

1. Introduction

In recent years, progress in microfabrication techniques has made it possible to design various kinds of quantum structures within which the wavelength of typical thermal carriers is comparable to or larger than the structure feature size. The thermal transport properties in quantum structures have attracted increasing attention [1]. The quantized thermal conductance with universal value ($\pi^2 k_B^2 T/3h$) by ballistic phonon in dielectric quantum wire with catenoidal contacts at very low temperature was predicted theoretically [2,3] and verified experimentally [4]. Quantized thermal conductance by electrons [5] and by photons [6,7] in quantum structures has also been found, and the universal thermal quantum is always $\pi^2 k_B^2 T/3h$. These results indicate that the thermal conductance quantum is independent of the types of energy carriers. Considering the fact that the ballistic phonons are primary energy carriers in semiconductor quantum wire at low temperatures, the thermal conductance by ballistic phonons attracts much attention. In ballistic phonon systems, when the feature size of quantum structure is smaller than the phonon mean free path in bulk material, the phonon scattering inside the structure and at the boundary has to be considered. In order to understand the effects of the structure on the phonon transport and thermal conductance, the thermal conductance properties have also been reported in various quantum structures such as one-dimensional chains [8,9], nanowires [10–13], nanotubes [14,15], graphene [16–22], quantum waveguides with abrupt junctions [23], rough surfaces [24], structural defects [25], and stub structures [26,27], and so on. Now, it is known that the thermal conductance is related with discrete vibrational modes including both propagating modes and evanescent modes [28]. At very low temperatures in one-dimensional (1D) or quasi-1D system, the lowest vibrational modes with different characteristics include four types of acoustic modes (namely the dilatational, torsional, and two types of flexural modes) and two types of optical modes (namely two shear modes) [2,29]. The quantized thermal conductance results from the fact that the stress-free boundary condition of ballistic phonon in quantum wire allows for the propagation of the acoustic mode with incident frequency $\omega = 0$, and that the scattering of the structure on the long-wavelength acoustic waves in the limit $T \to 0$ is very small. Although the geometry shape of the structures plays an important role in the phonon transport and thermal conductance, the thermal conductance in the limit $T \to 0$ is always kept to be the universal unit $\pi^2 k_B^2 T/3h$, regardless of geometry details. There exist

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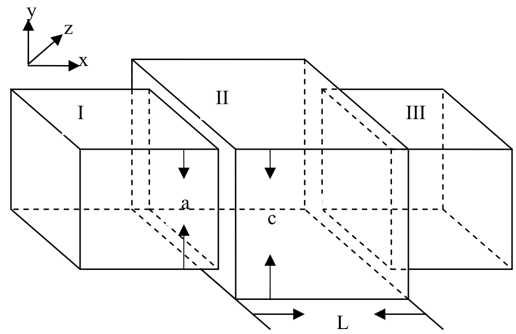

Fig. 1. Structure of quantum wire modulated with a quantum dot.

three types of acoustic modes in two-dimensional (2D) geometry: longitudinal polarized P mode, vertically polarized SV mode, and horizontally polarized shear SH mode with polarization directions being along the x, y, and z directions (z direction is perpendicular to the two-dimensional plane) [34], respectively. However, most of the previous studies focus on SH mode in 2D geometry [17,31–34], or the dilatational (longitudinal) mode in 1D geometry [27]. The phonon transport and thermal conductance for the other five vibrational modes such as torsional, two types of flexural modes and two types of shear modes have attracted very little attention due to the fact that it is difficult to calculate the ballistic thermal conductance of the phonon modes. Some studies [29,30] investigated the thermal conductance of the six lowest vibrational modes in catenoidal wires. These studies mainly focus on the dimension of the structure being of the order of micron.

In the present work, we study the transmission rates and thermal conductances contributed by the lowest six lattice vibrational modes in quantum wires modulated with quantum dot, as shown in Fig. 1. The results show that the thermal conductances contributed by different vibrational modes have different characteristics. It is necessary to consider the thermal conductances contributed by six types of vibrational modes in order to clarify the basic features of the thermal conductance at low temperatures, especially the quantum thermal conductance at very low temperatures.

This paper is organized as follows. In Section 2, a brief description of the model and the necessary formulae used in calculations are given. The numerical results are presented in Section 3 with analysis. Finally, we summarize our results in Section 4.

2. Model and method

The model structure shown in Fig. 1 is divided into three regions, the left region I is the heat reservoir with temperature T_1 for $x < 0$, the central region II is a quantum dot with length L for $0 < x < L$, and right region III is the heat reservoir with temperature T_3 for $x > L$. It is assumed that the temperature T_1 in region I is bigger than the temperature T_3 in region III and the difference δT ($\delta T = T_1 - T_3 > 0$) is very small. So we can adopt the mean temperature T $[T = (T_1 + T_3)/2]$ as the temperature of the structure in following calculations. In the structure considered here, the thermal transport direction is along the x direction from the left to the right, and the three regions are made of the same material. In this paper, we assume the contact between the quantum dot and the left or right lead is ideal and ignore the effect of contact resistance on phonon transport. Especially, we only focus on the effect of discontinuous interfaces on phonon transport and thermal conductance.

For the structure shown in Fig. 1, the thermal conductance K for each type of vibrational mode can be expressed as [2]:

$$K = \frac{\hbar^2}{k_B T^2} \sum_i \frac{1}{2\pi} \int_{\omega_i}^{\infty} \tau_i(\omega) \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2} d\omega. \tag{1}$$

Here $\tau_i(\omega)$ is the transmission rate of the mode i in region I at frequency ω across all the interfaces into the region III, ω_i is the cutoff frequency of the ith mode, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the temperature, and $\hbar$ is reduced Planck constant. The effect of scattering is introduced through the transmission rate $\tau_i(\omega)$, which determines the thermal conductance. The key issue in predicting the thermal conductance is to calculate the transmission rate $\tau_i(\omega)$.

For the present structure, the displacement field u of the dilatational mode in a quantum wire or quantum dot with a cross section A can be written as [35]:

$$\frac{1}{v_L^2} \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}. \tag{2}$$

Here, $v_L^2 = \frac{Y}{\rho}$. Y is the Young modulus of the material and ρ is the mass density. From the equation, we can get the dispersion relation $\omega = v_L k$. From the dispersion relation, it is known that the frequency ω linearly depends on the wave number k, which shows the lowest dilatational mode is acoustic mode. By the continuous condition of the displacement u and the stress $\partial u/\partial x$ at all the interfaces, we can obtain the transmission rate of the dilatational mode:

$$|\tau_D|^2 = \frac{(4A_1A_2)^2}{(A_1 + A_2)^4 + (A_1 - A_2)^4 - 2(A_1^2 - A_2^2)^2 \cos(2Lk)}. \tag{3}$$

The equation can be simplified as:

$$|\tau_D|^2 = \frac{16}{(\sqrt{A_1/A_2} + \sqrt{A_2/A_1})^4 + (\sqrt{A_1/A_2} - \sqrt{A_2/A_1})^4 - 2(A_1/A_2 - A_2/A_1)^2 \cos(2Lk)}. \tag{4}$$

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