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Different effect of evanescent modes on acoustic phonon transport in different types of a three-dimensional quantum wire

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ABSTRACT

By the use of the scattering matrix method, we investigate the effect of evanescent modes on acoustic phonon transport and thermal conductance in both convex and concave type three-dimensional quantum wire. Our results show that the evanescent modes can enhance the transmission coefficient and the thermal conductance in the concave type three-dimensional quantum wire. However, for the convex type three-dimensional quantum wire, the evanescent modes can play adverse effect on the phonon transport. When the length of scattering region is large enough, for all types of three-dimensional quantum wire, the influence of evanescent modes on phonon transport becomes very weak.

1. Introduction

In recent years, the heat transport by phonons in nanostructures has been attracting increasing attention. Up to now, many attractive investigations on heat transport have been reported in various kinds of nanostructures, such as thin film [1–3], superlattices [4–7], nanowires [8–16], and nanotube [17–25]. Recently, heat transport in the quantum waveguide structures has been investigated using the scattering matrix method [26–29]. Some interesting features are revealed, such as acoustic-phonon mode splitting behavior and the noninteger quantized thermal conductance in an asymmetric y-branch three-terminal junction [8], and phonon transmission and thermal conductance can be controlled by adjusting the parameters of the stub in a T-shaped waveguide structure [26], and the phonon cavity lying in a narrow constriction of a semiconductor nanowire can enhance the thermal conductance at very low temperatures [27], and the thermal conductance versus temperature is qualitatively different for the quantum waveguide with defects which consist of void or clamped material [28], and the thermal conductance of a cylindrical quantum structure can be efficiently tuned by modulating the radius, length of double quantum dots as well as the interval between double quantum dots [29]. It is well known that the thermal energy in the quantum structures is carried by a set of discrete phonon modes or vibrational modes due to transverse confinement. According to their propagating length along nanowire, the modes can be classified as propagating modes and evanescent modes. Propagating modes can propagate in total nanowire, but evanescent modes will gradually disappear in the nanowire. Several groups [30–33] have studied electronic states in mesoscopic structures; it is found that the evanescent modes are important to electron transmission in quantum wires with inhomogeneities. Similarly to the case of electrons, when the phonon is restricted to a quantum structure with inhomogeneity, evanescent modes will emerge from the scattering region in the quantum structure. In practicable calculations of the acoustic phonon transport and thermal conductance in the quantum structures, several evanescent modes have also been taken into account [8,9,11,12,26–29]. However, very few studies have been reported regarding the effect of evanescent modes on the acoustic phonon transport probability and thermal conductance in a three-dimensional quantum wire.

In this letter, we investigate the effect of evanescent modes on acoustic phonon transport and thermal conductance in different types of a three-dimensional quantum wire. Our results show that the evanescent modes can enhance the transmission coefficient and the thermal conductance in the concave type three-dimensional quantum wire. However, for the convex type three-dimensional quantum wire, the evanescent modes can play adverse effect on the phonon transport. When the length of scattering region is large enough, for all types of three-dimensional quantum wire, the influence of evanescent modes on phonon transport becomes very weak.

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This letter is organized as follows: Section 2 gives a brief description of the model and the formulas used in calculations. The calculated results are presented in Section 3 with discussions. Finally, a summary is made in Section 4.

2. Model and formalism

The model of the three-dimensional quantum wire (material is GaAs) shown in Fig. 1 is divided into three regions which compose the phonon channel, a_η and b_η ($\eta = 1$–3) denote the lateral widths of the corresponding region ξ, $\xi =$ I–III. The longitudinal length of region II is d. The main quantum waveguide consists of regions I and III, and the convex or concave section is made up of region II. It is assumed that the temperatures in regions I and III are T_1 and T_3, respectively, and the difference δT ($\delta T = T_1 - T_3 > 0$) is very small. So the mean temperature T [$T = (T_1 + T_3)/2$] can be adopted as the temperature of regions I and III in the following calculations. For the three-dimensional quantum wire depicted in Fig. 1, when mode mixing effects that could occur at boundaries and interfaces are ignored, there exist three types of acoustic modes: vertically polarized *SV* mode, horizontally polarized *SH* mode, and longitudinal polarized *P* mode, as expounded in the elasticity textbook by Graff [34]. Their polarization directions are along the x, y, and z directions, respectively. The previous letter [8] has investigated the effect of mode mixing between *SV* and *P* on the thermal conductance at low enough temperatures. The results show that at a low temperature, the effect of mode mixing on the thermal conductance is very small, and that the thermal conductance of the *SH* wave has similar features to those of the *P* (or *SV*) mode. So, in the letter, we only discuss the thermal conductance of *SH* mode. For the structure considered in Fig. 1, the expression of thermal conductance K can be written as [35]

$$K = \frac{\hbar^2}{k_B T^2} \sum_{mn} \frac{1}{2\pi} \int_{\omega_{mn}}^{\infty} \tau_{mn}(\omega) \frac{\omega^2 e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2} d\omega, \tag{1}$$

where $\tau_{mn}(\omega)$ is the energy transmission coefficient from mode (m, n) of region I at frequency ω across all the interfaces into the modes of region III, ω_{mn} is the cutoff frequency of the (m, n)th mode, $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the temperature, $\hbar$ and is Planck's constant. The effect of scattering is introduced through the transmission coefficient $\tau_{mn}(\omega)$, and the $\tau_{mn}(\omega)$ can be derived by using the scattering matrix method.

In this letter, the elastic model is employed to calculate the transmission coefficient $\tau_{mn}(\omega)$ of acoustic phonon. Our work focuses on *SH* mode polarized in the y direction. In the elastic approximation, the displacement fields of the *SH* mode is governed by a single scalar equation:

$$\frac{\partial^2 \psi}{\partial t^2} - v_{SH}^2 \nabla^2 \psi = 0, \tag{2}$$

where the *SH* wave velocity v_{SH} is related to the mass density ρ and elastic stiffness constant C_{44}, and

$$v_{SH} = \sqrt{C_{44}/\rho}. \tag{3}$$

Applying the stress-free boundary condition to each interface in the structure, i.e.,

$$n_0 \cdot \nabla \psi = 0, \tag{4}$$

where n_0 is normal to the corresponding interface, the phonon displacement field equations in the three regions can be expressed as

$$\psi^\xi(x, y, z) = \sum_{m=0}^{M^\xi} \sum_{n=0}^{N^\xi} \left[C^\xi_{mn} e^{ik^\xi_{mn} z} + D^\xi_{mn} e^{-ik^\xi_{mn} z}\right] \phi^\xi_{mn}(x, y), \tag{5}$$

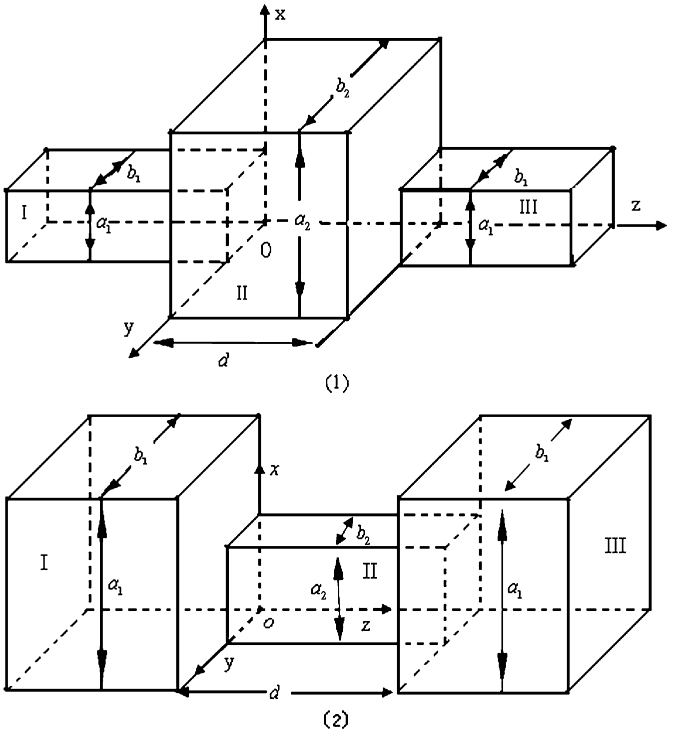

Fig. 1. Schematic illustration of three-dimension quantum wires for: (1) convex type with two bigger lateral widths; (2) concave type with two smaller lateral widths.

where C^ξ_{mn} and D^ξ_{mn} are constants to be determined by matching the boundary conditions. $\xi =$ I–III, $\phi^\xi_{mn}(x, y) = \phi^\xi_m(x)\phi^\xi_n(y)$ represents the orthogonal transverse mode (m, n) in region ξ. In region ξ,

$$\phi^\xi_n(x) = \begin{cases} \sqrt{\frac{2}{a_\eta}} \cos \frac{m\pi}{a_\eta} x & (m \neq 0), \\ \sqrt{\frac{1}{a_\eta}} & (m = 0); \end{cases} \tag{6}$$

and

$$\phi^\xi_n(y) = \begin{cases} \sqrt{\frac{2}{b_\eta}} \cos \frac{n\pi}{b_\eta} y & (n \neq 0), \\ \sqrt{\frac{1}{b_\eta}} & (n = 0); \end{cases} \tag{7}$$

the wave number k^ξ_{mn} in region ξ can be given by energy conservation condition,

$$k^\xi_{mn} = \sqrt{\frac{\omega^2}{v_{SH}^2} - \frac{m^2\pi^2}{a_\eta^2} - \frac{n^2\pi^2}{b_\eta^2}}. \tag{8}$$

Here, ω is the incident phonon frequency, $\eta = 1$–3, a_η and b_η are the lateral widths of region ξ, $v_{SH} = \sqrt{C_{44}/\rho}$ is the wave velocity of *SH* mode in the region ξ.

The matching conditions are determined by the requirement of continuity of the displacement ψ and the stress $C_{44}\partial\psi/\partial z$ at the interfaces I–II, and II–III. Then, we can derive the transmission coefficient $\tau_m(\omega)$ by using the scattering matrix method [36,37]. For further details of the method, see [26].

From Eq. (8), when $\omega < \sqrt{\frac{m^2\pi^2 v_{SH}^2}{a_\eta^2} + \frac{n^2\pi^2 v_{SH}^2}{b_\eta^2}}$, the wave vector k_{mn} is a purely imaginary number, and the corresponding mode is called evanescent mode. If $\omega \geqq \sqrt{\frac{m^2\pi^2 v_{SH}^2}{a_\eta^2} + \frac{n^2\pi^2 v_{SH}^2}{b_\eta^2}}$, the wave vector k_{mn} is a real number, and the corresponding mode is called propagating mode. Theoretically, the number of transversal modes