Available online at www.sciencedirect.com
SCIENCE DIRECT®
Physics Letters A 350 (2006) 302–308
PHYSICS LETTERS A
www.elsevier.com/locate/pla

Acoustic phonon transport through a double-bend quantum waveguide

Y. Ming *, Z.X. Wang, Z.J. Ding *

Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, 230026 Anhui, People's Republic of China

Received 17 August 2005; received in revised form 15 October 2005; accepted 17 October 2005

Available online 25 October 2005

Communicated by R. Wu

Abstract

In this work, using the scattering matrix method, we have investigated the transmission coefficients and the thermal conductivity in a double-bend waveguide structure. The transmission coefficients show strong resonances due to the scattering in the midsection of a double-bend structure; the positions and the widths of the resonance peaks are determined by the dimensions of the midsection of the structure. And the scattering in the double-bend structure makes the thermal conductivity decreases with the increasing of the temperature first, then increases after reaches a minimum. Furthermore, the investigations of the multiple double-bend structures indicate that the first additional double-bend structure suppresses the transmission coefficient and the frequency gap formed; and the additional double-bend structures determine the numbers of the resonance peaks at the frequency just above the gap region. These results could be useful for the design of phonon devices.

PACS: 63.22.+m; 73.23.Ad; 44.10.+i

1. Introduction

Since the discovery of the quantized electronic conductance phenomena [1,2], the double-bend electron waveguide has been investigated as a very important case. The problem was firstly studied by Weisshaar et al. [3] using mode-matching technique. The experiment work on the low temperature conductance of the double-bend waveguide was carried out by Wu et al. [4]. By using the recursive Greens function technique, Kawamura et al. [5,6] studied this double-bend waveguide again. All the works showed strong resonant transmission due to internal reflections in the special structure and Refs. [5,6] showed the "existence of an energy gap between the first and second subband threshold energies where the conductance is suppressed for multiple double-bend structures". Based on the property of the strong resonant transmission through the double-bend waveguide, Shi et al. [7] proposed a simple spin filter with which an extremely large spin current is expected.

Same as the electronic conductance, the thermal conductivity is also important for semiconductor nanostructures. For an ideal elastic beam at an enough low temperature, the thermal conductivity is dominated by the ballistic phonon and is quantized in a universal unit, $\pi^2 k_B^2 T/3h$, analogous to the well-known $2e^2/h$ electronic conductance quantum [8–10]. These predictions have been verified experimentally [11]. Since then, many works have been done to study the geometrical effects on the transmission of the acoustic phonon and the thermal conductivity through the quantum waveguide with various geometries [12–20]. But as an important case, the quantum waveguide with a double-bend structure has not been studied on the phonon transmission coefficients and thermal conductivity. Therefore, in this work, we calculate the phonon transmission coefficients and thermal conductivity in a double-bend quantum waveguide using the scattering-matrix method [21–25] and considering the stress-free boundary condition [15–20].

The organization of this Letter is as follows. In Section 2, we present the model and the numerical method briefly. The numerical results for a one double-bend structure are discussed in Section 3. In Section 4, the results of a two double-bend structures are presented. Finally, a summary is made in Section 5.

* Corresponding authors.
E-mail addresses: meanyee@mail.ustc.edu.cn (Y. Ming), zjding@ustc.edu.cn (Z.J. Ding).

0375-9601/$ – see front matter
doi:10.1016/j.physleta.2005.10.047

2. Model and formalism

The geometry of the double-bend quantum waveguide is sketched in Fig. 1. Regions-I and -III are the leads of the device; region-II is the midsection. The parameters of this device are W, L and D_1, which are the lateral width of the leads, the lateral width of the midsection and the longitudinal length of the midsection, respectively. We assume that the temperature in the two leads (regions-I and -III) are T_1 and T_2; and the temperature difference δT ($\delta T = T_1 - T_2 > 0$) between two leads is very small. The mean temperature T ($= (T_1 + T_2)/2$) may then be adopted as the temperature of two leads. In this work, we choose the same thickness for the three regions and let the thickness smaller than the other two dimensions and also than the wavelength or the coherence length of the elastic waves; there is no mixing of the z modes and a two-dimensional calculation is then adequate [8–10,15]. For the imperfect contact at the regions-I and -III, the thermal conductance K at temperature T is given by [8,15]

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

where $\tau_m(\omega)$ is the transmission coefficient from mode m of region-I at frequency ω across all the interfaces into the modes of region-III; ω_m is the cutoff frequency of the mth mode; $\beta = 1/(k_B T)$, k_B is the Boltzmann constant, T is the temperature; and $\hbar$ is the Planck's constant. It can be seen from Eq. (1) that the central issue of the problem is to obtain the transmission coefficient, $\tau_m(\omega)$.

We consider the scalar model for the elastic wave; the model for thin geometry at low temperature is used so that the calculation is two-dimensional. Here, we treat the simplest case for a horizontally polarized wave (SH) (polarized along the z direction) propagating in the x-direction. So the wave equation of the displacement field u is

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

where v_{SH} is related to the mass density ρ and elastic stiffness constant C_{44} by

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

The stress-free boundary conditions at the edges require $\hat{n} \cdot \nabla u = 0$, where $\hat{n}$ is the unit vector normal to the edge. For the double-bend structure depicted in Fig. 1, the solution to Eq. (2) in region-ξ (regions I, II and III) can be expressed as

$$u^\xi(x, y) = \sum_{m=0}^{N} \left[A_m^\xi e^{ik_m^\xi (x - x_\xi)} + B_m^\xi e^{-ik_m^\xi (x - x_\xi)} \right] \phi_m^\xi(y), \tag{4}$$

where x_ξ is the reference coordinate along the x-direction in region-ξ; k_m^ξ is the wavenumber of the transmitted and reflected waves in region-ξ, giving by the energy conservation condition

$$\omega^2 = {k_m^\xi}^2 {v_{SH}^\xi}^2 + m^2 \pi^2 {v_{SH}^\xi}^2 / W_\xi^2, \tag{5}$$

with W_ξ the transverse dimension of region-ξ; $\phi_m^\xi(y)$ represents the transverse wavefunction of acoustic mode-m in region-ξ,

$$\phi_m^{I} = \begin{cases} \sqrt{\frac{2}{W}} \cos \frac{m\pi}{W} y & (m \neq 0), \\ \sqrt{\frac{1}{W}} & (m = 0), \end{cases} \tag{6}$$

$$\phi_m^{II} = \begin{cases} \sqrt{\frac{2}{L}} \cos \frac{m\pi}{L} y & (m \neq 0), \\ \sqrt{\frac{1}{L}} & (m = 0), \end{cases} \tag{7}$$

$$\phi_m^{III} = \begin{cases} \sqrt{\frac{2}{W}} \cos \frac{m\pi}{W} (y - L) & (m \neq 0), \\ \sqrt{\frac{1}{W}} & (m = 0). \end{cases} \tag{8}$$

In principle, the sum over m in Eq. (4) includes all propagating modes and evanescent modes (imaginary k_m^ξ). However, in the practical calculation, besides all the propagating modes we only take a same limited number of evanescent modes into account to meet the desired precision for each region in a double-bend structure. The boundary matching conditions require the continuity of the displacement u and the stress $C_{44}\partial u/\partial x$ at the interface of regions-I and -II and the interface of regions-II and -III. So we can obtain the equations for the coefficients in Eq. (4). Rewriting the resulted equations in the form of matrix, we can derive the transmission coefficient, τ_m, by the scattering matrix method [21–25].

In the calculations, we employ the following values of elastic stiffness constant and the mass density [26]: $C_{44}(\text{GaAs}) = 5.99$ (10^{10} N m^{-2}) and $\rho(\text{GaAs}) = 5317.6$ (kg m^{-3}), and choosing $W = 10$ nm.

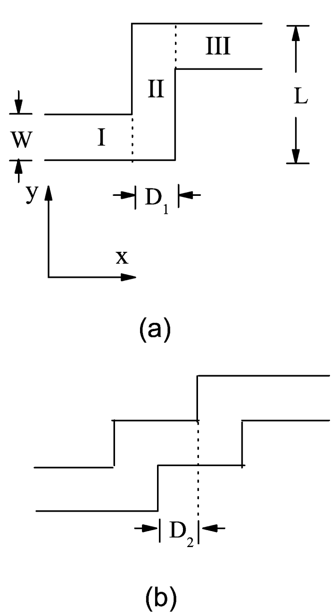

Fig. 1. (a) Double-bend waveguide with lead width W, lateral length L, and longitudinal length D_1. (b) Two double-bend waveguides in a series with the longitudinal length D_2.

3. Numerical results for a one double-bend structure

For acoustic phonon mode, the stress-free boundary condition allows acoustic waves propagate through the structure in