Effect of defects on the thermal conductivity in a nanowire

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We investigate the effect of defects on the low temperature thermal conductance in nanowire structure by using the scattering-matrix method. It is found the behavior of the thermal conductance versus temperature is qualitatively different for different types of defects. When the defect is void, the universal quantum thermal conductance and the decrease of the thermal conductance at low temperature can be clearly observed. However, when the structural defect consists of clamped material, the quantized thermal conductance cannot be observed, and the thermal conductance increases monotonically with increasing temperature.

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I. INTRODUCTION

There is currently increasing interest in heat transport associated with phonons in semiconductor nanostructures because technological advances in nanoscale lithography and atom-layer epitaxy enable us to obtain various semiconductor nanostructures within which the wavelength of a typical thermal phonon comparable to or larger than the structure feature size. The phonon thermal conductance in various kinds of nanostructures such as quantum wells,[1] superlattices,[2–5] nanowires,[6–12] one-dimensional glass,[13] and nanotubes[14] were reported. Several groups[15,16] have derived the expressions of thermal conductance for ballistic phonon transport at a low enough temperature in an ideal elastic beam, and found that the thermal conductance at low temperature is quantized in a universal unit $\pi^2 k_B^2/3h$, analogous to the well-known $2e^2/h$ electronic conductance quantum. These predictions have been verified by experiment.[17] However, the experiment showed that the value of K/T unexpectedly decreases as the temperature increases in the range of 0.08 to 0.2 K. It is suggested that the likely causes of the decrease of the thermal conductance in low temperatures are the imperfect acoustic coupling between the wire and the reservoirs, the scattering due to rough surfaces, or the scattering by the defects in the structure. Using the Landauer formulation of transport theory, Rego and Kirczenow[15] predicted the existence of a universal quantum of thermal conductance in the dielectric quantum wires with catenoid contacts between the wire and the reservoirs, but without referring to the decrease of the thermal conductance in low temperature. Santamore and Cross,[18] based on a Green's function formalism, investigated the effect of surface roughness on the universal thermal conductance in a dielectric quantum wire at low temperature. They showed that the presence of rough surface significantly decreases the thermal conductance below the universal level. Lu *et al.*[19] calculated the longitudinal acoustic mode contribution to the thermal conductance by taking into account the interface scattering due to the surface roughness and catenoid contacts, and observed an obvious reduction of the lattice thermal conductance at sufficiently low temperature.

To our knowledge, however, the influence of defects on the thermal conductance has not been reported so far. Usually, nanostructures such as nanowires are not ideal with both natural and artificial defects. Defects can lead to the localization of acoustic modes in the vicinity of the defects.[20] This will cause the additional scattering to the transport phonons, which results in the change of the thermal conductance for ballistic phonon transport. In the present work, we calculated the thermal conductance in a nanowire with typical structural defects consisting of void or clamped material. In such a quantum structure, there exist three types of acoustic modes: longitudinal polarized **P** mode, vertically polarized **SV** mode, and horizontally polarized shear **SH** mode, as expounded by Graff.[21] Considering the fact that our work focuses on the acoustic phonon thermal transport at low enough temperature, where only several lowest modes can be excited and the most contribution to the thermal conductance comes from zero mode. In this case the effect of the mode mixing on the thermal conductance is small.[22] So in the present paper, we only discuss the thermal conductance of **SH** mode, and we think that this could clarify the basic features of the thermal transport at low temperature in this type of structure.

This paper is organized as follows: Sec. II gives a brief description of the model and the formulas used in calculations. The calculated results are presented in Sec. III with analyses. Finally, a summary is made in Sec. IV.

II. MODEL AND FORMALISM

We model the geometry as illustrated in Fig. 1. For simplicity, we assume here that the structure regions I, II, and III have the same thickness, and are small with respect to the other dimensions and also to the wavelength of the elastic waves, so that the horizontally polarized shear **SH** mode is decoupled from the phonon modes polarized in the *x*-*y* plane.[21] In addition, we assume that the temperatures in regions I and III are T_1 and T_2, respectively; and the temperature difference $\delta T(\delta T = T_1 - T_2 > 0)$ between regions I and III is small. So we can adopt the mean

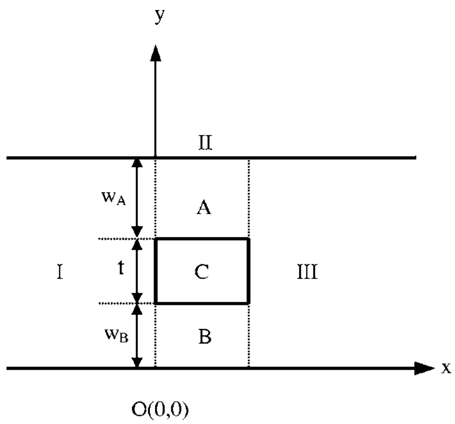

FIG. 1. Schematic illustration of a nanowire with defect region C. The structure is divided into three regions I, II, and III. Regions I and III are semi-infinite incident and outgoing leads, respectively. Region II consists of three parts A, B, and C. Parts A and B are tunnel regions with widths w_A and w_B, respectively; while part C is a structural defect with the width t. The length of parts A, B, and C is d. Here, we consider two typical defects: void and clamped material. The rest part of the whole structure consists of GaAs material.

temperature $T[T=(T_1+T_2)/2]$ as the temperature of regions I and III in our calculations. For the structure considered here, the formula for the thermal conductance can be expressed by:[23]

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

where $\tau_m(\omega)$ is the energy transmission coefficient from mode m of region I at frequency ω across all the interfaces into region III. A central issue in calculating the thermal conductance is then to calculate the transmission coefficient $\tau_m(\omega)$. In this paper, we employ the elastic model to calculate the transmission coefficient of the acoustic phonon. Our work focuses on **SH** mode propagating in the x direction. In the elastic approximation, the elastic equation of motion for longitudinal wave is

$$\frac{\partial^2\psi}{\partial t^2}-v^2\nabla^2\psi=0, \qquad (2)$$

where $v=\sqrt{C_{44}/\rho}$ is sound velocity of **SH** mode related to the mass density ρ and elastic stiffness constant C_{44}. The solution to Eq. (2) in region I can be written as

$$\psi^{\mathrm{I}}(x,y)=\sum_{m=1}^{N_1}[A_m^{\mathrm{I}}e^{ik_m^{\mathrm{I}}x}+B_m^{\mathrm{I}}e^{-ik_m^{\mathrm{I}}x}]\phi_m^{\mathrm{I}}(y), \qquad (3)$$

where $\phi_m^{\mathrm{I}}(y)$ represents the transverse wave function of acoustic mode m in region I. Employing the stress free boundary condition $\hat{n}.\nabla\phi=0$ at the edges, we have

$$\phi_m^{\mathrm{I}}(y)=\begin{cases}\sqrt{2/w}\cos\frac{m\pi}{w}y & (m\neq 0)\\ \sqrt{1/w} & (m\equiv 0).\end{cases} \qquad (4)$$

Note that this stress free boundary condition allows the propagation of zero acoustic mode with $\omega(k\rightarrow 0)\rightarrow 0$, which is of greater practical interest than the hard boundary condition. The effects of both stress-free and hard boundary conditions on the propagation of zero acoustic mode in nanowire have already been discussed by Cross and Lifshitz.[23] k_m^{I} can be given by the energy conservation condition

$$k_m^{\mathrm{I}}=\sqrt{\omega^2/v_{\mathrm{I}}{}^2-m^2\pi^2/w^2}. \qquad (5)$$

Here, ω is the incident phonon frequency. For region II, we have

$$\psi^{\mathrm{II}}(x,y)=\sum_{n=1}^{N_2}[C_n^A e^{ik_n^A x}+D_n^A e^{-ik_n^A x}]\phi_n^A(y)+\sum_{n=1}^{N_2}[C_n^B e^{ik_n^B x}+D_n^B e^{-ik_n^B x}]\phi_n^B(y). \qquad (6)$$

If part C is void, stress-free boundary condition should be introduced at the interfaces between parts A and C, as well as between B and C, then the transversal wave functions $\phi_n^A(y)$ in part A ($w_B+t\leq y\leq w$), and $\phi_n^B(y)$ in part B ($0\leq y\leq w_B$) can be expressed as

$$\phi_n^A(y)=\begin{cases}\sqrt{2/w_A}\cos\frac{n\pi}{w_A}(y-w) & (n\neq 0)\\ \sqrt{1/w_A} & (n\equiv 0),\end{cases} \qquad (7)$$

and

$$\phi_n^{\mathrm{B}}(y)=\begin{cases}\sqrt{2/w_B}\cos\frac{n\pi}{w_B}y & (n\neq 0)\\ \sqrt{1/w_B} & (n\equiv 0).\end{cases} \qquad (8)$$

The wave number is

$$k_n^{\xi}=\sqrt{\omega^2/v_{\xi}^2-n^2\pi^2/w_{\xi}^2}\quad(\xi=A,B). \qquad (9)$$

If part C is clamped material, the wave functions in parts A and B will suffer the hard-wall boundary condition at the interface between parts A and C, as well as between B and C. The transversal wave functions $\phi_n^A(y)$ and $\phi_n^B(y)$ in part B are, respectively, expressed as

$$\phi_n^A(y)=\sqrt{2/w_A}\cos\frac{(2n+1)\pi}{2w_A}(y-w), \qquad (10)$$

and

$$\phi_n^B(y)=\sqrt{2/w_B}\cos\frac{(2n+1)\pi}{2w_B}y. \qquad (11)$$

The wave number should be

$$k_n^{\xi}=\sqrt{\omega^2/v_{\xi}^2-(2n+1)^2\pi^2/4w_{\xi}^2}\quad(\xi=A,B). \qquad (12)$$

In region III, the solution in Eq. (2) can be written as

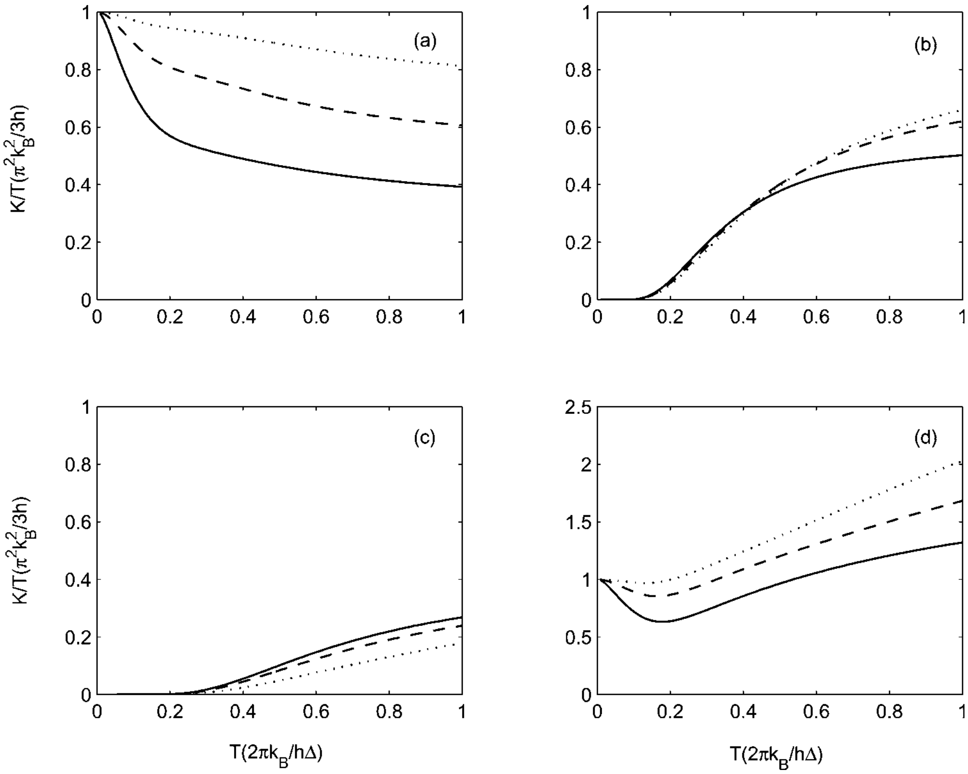

FIG. 2. The thermal conductance divided by temperature K/T, which is reduced by the zero-temperature universal value $\pi^2 k_B^2/3h$, as a function of the reduced temperature $k_BT/\hbar\Delta$ for different width t, where $\Delta=\omega_{n+1}-\omega_n=\pi v/w_I$ (v is the acoustic wave velocity in region I). Here, the defect C is void. (a)–(c) correspond to K/T of modes 0, 1, and 2, respectively, and (d) corresponds to the total K/T. Note that the total K/T should include the contributions of all the propagation modes. By our calculations, however, only the first six modes can make their contributions to the total thermal conductance for the explored temperature scope. The dotted, dashed, and solid curves correspond to $t=30$, 50, and 70 nm. Here, we take $w_a=w_b$, $t+w_a+w_b=100$ nm, and $d=50$ nm.

$$\psi^{\mathrm{III}}(x,y)=\sum_{m=1}^{N_1}\left[A_m^{\mathrm{III}}e^{ik_m^{\mathrm{III}}x}+B_m^{\mathrm{III}}e^{-ik_m^{\mathrm{III}}x}\right]\phi_m^{\mathrm{III}}(y), \qquad (13)$$

where $\phi_m^{\mathrm{III}}(y)=\phi_m^{\mathrm{I}}(y)$, $k_m^{\mathrm{III}}=k_m^{\mathrm{I}}$.

Note that the sum over n or m includes all propagating and evanescent modes (imaginary k). However, in the real calculations, we take all the propagating modes and several lowest evanescent modes into account to meet the desired precision. The connection between the coefficients in any two adjacent regions can be obtained by use of the boundary matching, the displacement ϕ, and the strain $C_{44}\partial\phi/\partial x$ are continuous at each interface. Then we can derive the transmission coefficient τ_m by using the scattering matrix method.[24] In the calculations, we will employ those values of dielectric constants and density of GaAs referred to Ref. 20.

III. NUMERICAL RESULTS AND DISCUSSION

We first explore the effect of void defect on the reduced thermal conductance for different width t in Fig. 2. For the structure discussed here, the stress-free boundary condition is applied in the leads A and B in region II. From the figure, it is clearly seen that as the temperature $T\to 0$ only the zero mode contributes to the thermal conductance and K/T approaches the ideal universal value $\pi^2k_B^2/3h$. Zero mode with transversal index $n=0$ propagating through the structure is the peculiarity of the elastic wave, which results from the stress-free boundary condition of acoustic phonon allowing the propagation of the mode with $\omega=0$. We also find from Fig. 2(a) that the reduced thermal conductance at $T\to 0$ is independent of the width t. This indicates that the scattering of the defect on the long-wavelength acoustic waves with $\omega\to 0$ and $k\to 0$ is very small. With an increase in the temperature, T, the modes with the higher transverse modes $n(n>0)$ such as modes 1 [see Fig. 2(b)] and 2 [see Fig. 2(c)] start to contribute to the thermal conductance, and their reduced thermal conductance K/T is increased, which indicates that the conductance K of the higher modes is proportional to $T^\gamma(\gamma>1)$. However, the value K/T of zero mode decreases as the temperature is increased. This means that the conductance K of the zero mode is proportional to $T^\gamma(0<\gamma<1)$. These results indicate that the effect of the structural defect on the thermal conductance of the zero mode is different from that of the higher modes. It is the decrease of the K/T of the zero modes that leads to the decrease of the value of the total K/T in the very low temperature range [see Fig. 2(d)]. This view seems to agree with the experimental results qualitatively,[17] where also observed is a similar decrease in the thermal conductance below the universal value. Moreover, from Fig. 2(a), it is clearly seen that with the increase of the thickness of the defect C, the value K/T of zero mode decreases. However, we can find from Fig. 2(b) that the value K/T of the mode 2 at $t=70$ nm is bigger than that at $t=50$ nm through the temperature range explored, namely, the value K/T of the mode 1 is bigger at smaller thickness t for a certain temperature range. This can be understood from a physical point of view. In general, the bigger the thickness t, the stronger the scattering of the defect C on the phonon modes, the smaller the value K/T. However, the reverse cases may occur due to the coupling between the two leads A and B, similar to the case of the resonant electron transmission through a single barrier. Of course, the coupling strength is related to the index of the modes and temperature.

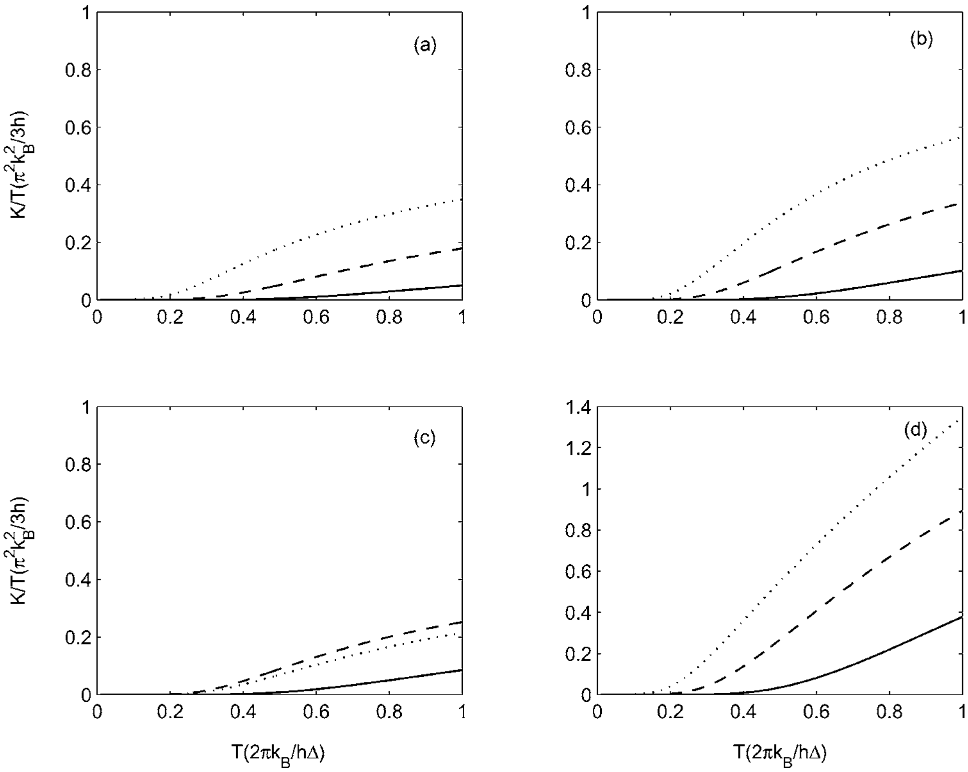

FIG. 3. The thermal conductance divided by temperature K/T, which is reduced by the zero-temperature universal value $\pi^2 k_B^2/3h$, as a function of the reduced temperature $k_B T/\hbar\Delta$ for different width t. Here, the defect C is clamped material. The structural parameters and explanations for curves are the same as for Fig. 2.

When the defect C consists of clamped material, where hard-wall boundary condition should be satisfied at the boundaries between the lead A and defect, as well as between lead B and defect in region II, the results, described in Fig. 3, is substantially different from those given in Fig. 2. Firstly, the universal quantum thermal conductance at $T \to 0$ is not observed. There exists a threshold temperature where the zero mode can be excited, and the value K/T of the zero mode is increased with the temperature, and has similar temperature dependence to that of modes 1 or 2, namely, $T^{\gamma}(\gamma > 1)$. From the formula (12), it is known that the threshold frequency of the zero mode is not zero, thus this mode can be excited only in the temperature higher than the threshold temperature. This results from the hard-wall boundary condition at the boundary between the leads A (or B) and C due to the defect C consisting of clamped material. Moreover, from Fig. 3(d), we do not observe the decrease of the total K/T in low temperature region. The influence of the type of defects on the thermal conductance is obvious. It is, therefore, known that the universal quantum thermal conductance can be observed only under condition of the ballistic boundary, where zero mode can be excited at $T \to 0$. As to the decrease of the total K/T in the low temperature region results from the scattering by the defects on zero mode as discussed here, the scattering due to rough surfaces,[18,19] and the imperfect acoustic coupling between the wire and the reservoirs.[24] Compare Fig. 3(d) with Fig. 2(d), it can be found that the void defect is more favorable for the thermal transmission of the acoustic phonon.

IV. SUMMARY

In conclusion, our results show an interesting physical effect: The behavior of the thermal conductance is qualitatively different for the different type of the defects. When the defect is void, where the same stress-free boundary condition for acoustic mode was used for the scattering region II, and the incident and outgoing leads I and III, ballistic transport for the $m=0$ phonon mode is possible. The thermal conductance reaches the universal quantum thermal conductance at zero temperature, and then decreases with the increase of the temperature. For higher temperature where the higher transverse modes $n(n>0)$ such as mode 1 start to contribute to the thermal conductance, the thermal conductance behaves as $T^{\gamma}(\gamma > 1)$. However, when the structural defect is consisted of clamped material, where the hard-wall boundary condition was applied between structural defect and leads, the thermal conductance is zero at zero temperature and it increases monotonically with temperature.

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