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Disorder-induced enhancement of the thermoelectric efficiency in diameter-modulated nanowires

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ABSTRACT

Nanowires have better thermoelectric performance than their bulk counterparts. It has been predicted that the thermoelectric efficiency of nanowires can be further enhanced when their diameter is modulated. Here, we report on the effect of disorder in the nanowire modulation profile. Our calculations on the electron and phonon transport properties showed that disorder can induce a significant enhancement of the thermoelectric efficiency due to the very big decrease of the phonon thermal conductivity. It is pointed out that the amount of disorder present in the geometry of the nanowire is critical. It is shown that adequate disorder can significantly limit the phonon propagation while preserving sufficient electron propagation and high power factors. Our findings provide design guidelines for nanostructures with enhanced thermoelectric properties that could lead to novel devices for efficient thermal to electrical energy conversion.

1. Introduction

A good thermoelectric material requires low thermal conductivity to minimize thermal leakage from the hot to the cold contact. Moreover, it requires high electrical conductivity and high Seebeck coefficient. To accomplish all these requirements simultaneously is a difficult and challenging task. Nanostructures are considered promising for manipulating electrons and phonons in order to achieve better thermoelectric performances. In nanostructures, both electron and phonon properties are modified due to size effects. In addition, the effects of the nanostructure on the electron and phonon transport properties are expected to be distinct because the characteristic lengths of the two types of carriers are different [1,2].

Nanowires are considered very promising materials for enhancement of the thermal to electrical energy conversion efficiency in a controllable way and amenable to devices. Considerably high values of the thermoelectric figure of merit have been predicted in very thin wires [3–5] due to expected enhancement of the power factor by quantum confinement and also due to the reduction of the lattice thermal conductivity by boundary scattering [6–10], phonon confinement [11–14] and modification of the phonon energy spectra [15–17]. Very low thermal conductivities, close to the amorphous limit value, were measured [18] in Si nanowires of diameters ranging between 20 and 150 nm after chemical etching and they were attributed to phonon scattering by surface roughness. The effect of surface roughness in reducing the thermal conductivity has been, thereafter, explored by several researchers using various techniques. It has been confirmed that surface roughness causes a decrease in the thermal conductivity [19–22]. Nevertheless, it has been concluded that the drastic decrease of the thermal conductivity cannot be attributed to surface roughness [21,22] and should be connected with modification of the phonon states [23,24], This has been become evident in molecular dynamics calculations on Si nanowires [24] where a decrease of the phonon conductivity by more than one order of magnitude was found when a combination of surface ripples and core defects was assumed than when only typical surface roughness was considered. It has been additionally pointed out that excess surface roughness would deteriorate the electrical conductivity [25]. Enhanced electron scattering has also been shown to limit the thermoelectric performance of electrons in very thin wires [26,27].

As an alternative to the decrease of the wire diameter in order to achieve enhanced thermoelectric performance, we have proposed to modulate the wire diameter [28,29]. Enhanced electron thermoelectric properties [29] and reduced thermal conductivities have been calculated [30–34] in the ballistic transport regime. This behavior is attributed to the modification of the energy dependence of the transmission coefficient of both types of carriers (electrons of phonons) due to the modification of the carriers' energy states in the modulated nanowires. Similar behavior is to be expected in the diffusive transport regime and this has been indeed

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recently reported for the phonon conductivity [35,36]. In both of the two transport regimes, electron and phonon transport properties depend on the structure of the energy states contributing to transport. Based on this dependence, low-dimensional nanostructures have been evaluated against their thermoelectric performance [1,37]. In heterostructures superlattices [1,38,39], in heterowires [40] and in Si_xGe_{1-x} [41] nanowires an increase of the ZT was predicted due to the electron mini-band conduction and the enhanced scattering.

For thermoelectric applications, it is very crucial to optimize the transport properties of electrons and phonons simultaneously in the same structure. Here, we explore the effect of the nanowire geometry modulation on electrons and phonons in the same structures in order to identify possibilities for optimal thermoelectric performance. We have worked in the ballistic transport regime where the effect of the modulated geometry of the nanowire is directly connected to the transport coefficients though the energy dependence of the transmission coefficient. Our conclusions provide guidance for the diffusive transport regime.

The ballistic transport regime holds at low temperatures where the carriers' characteristic lengths are longer or comparable to the characteristic dimensions of the structure. Depending on the material, this regime can hold in low-dimensional structures with characteristic dimensions of several nanometers. Here we restrict to temperatures, $T \leqslant 10$ K where ballistic transport can be assumed for GaAs. In this temperature range, the phonon mean free path is of the order of mm [2,42,43] and phonon transport can be considered ballistic in nanowires with perfect boundaries and length of several μm [44]. Moreover, the phonon coherence length varies from 100 nm at $T = 1$ K to 10 nm at $T = 10$ K [42] and interference effects are expected in the energy dependence of the transmission coefficient of diameter-modulated nanowires for the modulation variation within the order of 10 nm that has been considered here. On the other hand, the electron mean free path can be of the order of 100 nm–1 μm in high mobility materials [45–49]. Indeed, ballistic nanowires have been fabricated and characterized in the last years [50–54]. Our work provides physics insight that could be useful in interpreting available low-temperature observations and hopefully inspire new experiments.

The structure of the paper is: the theoretical model is described in Section 2, the results are given and discussed in Section 3. Finally, main conclusions are drawn in Section 4.

2. Theoretical model

The thermoelectric efficiency is measured by the dimensionless figure of merit:

$$ZT = \frac{S^2 GT}{\kappa} \tag{1}$$

where G is the electron conductance, S is the thermopower, κ is the thermal conductance and T is the absolute temperature. The thermal conductance consists of two contributions: the electron thermal conductance κ_e and the phonon thermal conductance κ_{ph}. In the ballistic transport regime, the transport coefficients are determined by the carriers' transmission coefficients.

The electron transport coefficients are given by the following standard formalism:

$$G = -\frac{2e^2}{h}\int dE\ T_e(E)\frac{\partial f}{\partial E} \tag{2}$$

$$S = -\frac{1}{eT}\frac{\int dE(E-E_F)T_e(E)\frac{\partial f}{\partial E}}{\int dE\ T_e(E)\frac{\partial f}{\partial E}} \tag{3}$$

$$K = \frac{2e^2}{h}\frac{1}{e^2T}\int dE(E-E_F)^2 T_e(E)\frac{\partial f}{\partial E} \tag{4}$$

$$\kappa_e = -K - S^2 GT \tag{5}$$

where $T_e(E)$ is the electron transmission coefficient. The symbol f denotes the Fermi distribution function and E_F is the Fermi energy.

The phonon thermal conductance is given by the following expression:

$$\kappa_{ph} = \frac{\hbar^2}{k_B T^2}\sum_m \frac{1}{2\pi}\int_{\omega_m}^{\infty} T_{ph}^m(\omega)\frac{\omega^2 e^{\hbar\omega/k_BT}}{\left(e^{\hbar\omega/k_BT}-1\right)^2}d\omega \tag{6}$$

where ω_m is the cut-off frequency of the mth mode and $T_{ph}^m(\omega)$ is the transmission coefficient for phonon mode m and phonon frequency ω. The integration is over the frequency of the modes m propagating in the structure. At low temperatures that are considered here, the upper end of integration is well below the Debye energy. Optical phonons have higher energies and they are not excited. Only acoustic phonons contribute to the thermal conductivity.

The total phonon transmission coefficient T_{ph} is then calculated by

$$T_{ph} = \sum_m T_{ph}^m(\omega) \tag{7}$$

The transmission coefficients for electrons $T_e(E)$ and phonons $T_{ph}^m(\omega)$ are calculated using the scattering matric method [55,30,32]. The results shown here are representative for the involved physics. Dots have been selected, for illustration purposes, to represent the nanowire modulating unit. The parameters for GaAs have been used and the characteristic dimensions of a modulated nanowire are: the thick straight part of the wire is 50 nm, the dots are 35×20 nm and the constrictions between the dots are 10×5 nm. The '*distorted SL*' consists of a periodic sequence of non-identical dots. Here it is illustrated the case of 3 non-identical dots: 35×20, 45×20, 20×20 nm has been considered. The '*disordered SL*' consists of an array of non-identical dots with the widths of the dots varied randomly. Here it is illustrated the case of 20 dots with widths varying randomly within the range (15–45 nm). The results of the calculations do not depend on the lengths of the ending parts of the nanowire with constant width (50 nm) or on the length of periodically modulated nanowires.

3. Results and discussion

The transport coefficients are directly related to the energy dependence of the carriers' transmission coefficient thought the nanowire. For this reason, we start our discussion with the electron and phonon transmission coefficients.

In the case of a uniform straight nanowire, the electron transmission coefficient $T_e(E)$ is a step-like function of the electron energy. Each new step corresponds to a new occupied energy subband. The transmission probability is finite above a threshold that lies at the minimum of the first energy subband. In the case of a diameter-modulated nanowire, $T_e(E)$ deviates from the simple step-like form and consists of transmission resonances, transmission bands and transmission gaps, as shown in Fig. 1a for representative cases of diameter-modulated nanowires by: a single dot, by three identical dots and by five identical dots. The detailed structure of the transmission coefficient is the outcome of interference between propagating waves and resonance states of the modulating units [28]. The transmission resonances correspond to quasi-bound electron states of the modulating dots. For a periodic sequence of multiple dots, coupling between the quasi-bound states of the dots that are close in energy results in the formation of narrow propagation bands. At electron energies above the