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On the dependence of the thermal conductivity of width-modulated nanowires on the number of modulations

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Abstract. Our previous Monte Carlo simulations on the thermal conductivity of width-modulated nanowires indicated two distinct dependences of the decrease of the thermal conductivity κ relative to that of the non-modulated nanowire: (i) in the case of multiple constrictions κ scales with the nanowire transmissivity, (ii) in the case of a single constriction κ is determined by the ballistic constriction resistance. Here, we report on the transition between the two regimes. We discuss the thermal conductivity of width modulated nanowires as a function of the number of modulations. Phenomenology has been derived to interpret the MC simulations.

1. Introduction

Controlling the heat transfer is highly required in order to increase the efficiency of many applications in thermoelectrics, optoelectronics, nanoelectronics etc. Understanding the thermal conductivity of nanostructures is therefore a major research issue of scientific and technological interest. In nanostructures, nanoscale non-uniformity may cause phonon modification and phonon scattering that drastically affect the thermal conductivity. It is important to understand the dependence of the thermal conductivity on the underlying mechanisms. Our work aims to contribute to this need.

Porous materials and low-dimensional structures with characteristic dimensions above the quantum confinement regime, show reduced thermal conductivity due to enhanced phonon boundary scattering [1-5]. Width-modulated nanowires have been previously proposed as efficient thermoelectric materials [6-7]. It has been theoretically predicted that the transport properties of electrons and phonons are modified resulting in enhanced thermal to electrical energy conversion efficiency. In the quantum confinement regime, the phonon transmission coefficient and phonon energy states are modified so that the thermal conductivity decreases [8-10]. Above the quantum



confinement regime, the thermal conductivity of modulated nanowires was studied within the kinetic theory for phonons using an approximate model for boundary scattering [11]. A big reduction of the thermal conductivity was found due to enhanced boundary scattering and the decrease of the phonon transmissivity by the nanowire width-modulation. Phonon Monte Carlo (MC) simulations confirmed this evidence [12]. In addition they provided further insight and more quantitative description because this method is free of assumptions on the boundary scattering [12,13].

Our previous MC simulations on the thermal conductivity of width-modulated nanowires [12] indicated two distinct dependences of the decrease of the thermal conductivity κ relative to that of the non-modulated nanowire: (i) in the case of multiple constrictions κ scales with the phonon transmissivity, (ii) in the case of a single constriction κ is determined by the ballistic constriction resistance. Here, we report on the transition between the two regimes. We discuss the thermal conductivity of width modulated nanowires as a function of the number of modulations. Phenomenology has been derived to interpret the MC simulations.

2. Methodology and results

We have performed phonon MC simulations for the phonon transport using a previously developed simulation tools. The numerical method is extensively described in [12,14,15]. It lies on the resolution of the Boltzmann transport equation in the frame of the relaxation time approximation. Silicon dispersion properties have been used for the sampling of phonon frequency and group velocity, as well as for the calculation of the scattering relaxation times. The characteristic relaxation time is given according to the ‘Matthiessen’ summation rule. It takes into account: normal (N), umklapp (U) and impurity (I) scattering rates according to Holland [16] formalism. Here, we present simulations at room temperature. Diffusive boundary scattering has been assumed. At room temperature, the phonon’s wavelength is about 1 nm, depending on the way it is evaluated. Thus, the specularity parameter ($p = \exp(-16\pi^3\delta^2/\lambda^2)$, where δ is the roughness parameter and λ is the wavelength) is close to 0, meaning that every single reflection is diffuse.

The thermal conductivity of a nanowire with width modulated by a constriction is lower than that of a non-modulated nanowire [12]. This is to be expected since the constriction introduces extra boundary scattering. The thinner is the constriction the bigger is the decrease of the thermal conductivity. This dependence was found for all nanowire lengths as shown in Figure 1a, where the thermal conductivity is plotted as a function of the nanowire length for different constriction widths.

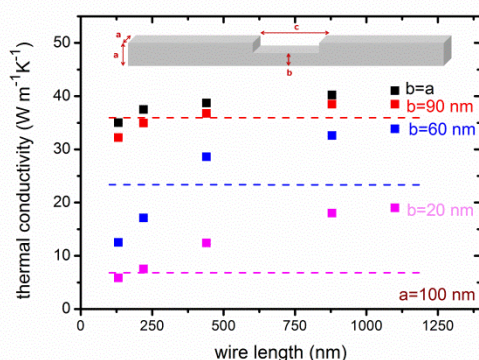


Figure 1. The thermal conductivity of a nanowire modulated by a single constriction versus the nanowire length for various values of the constriction width b (squares). The length of the constriction is $c=10$ nm. Periodically modulated nanowires with the same parameters a and b

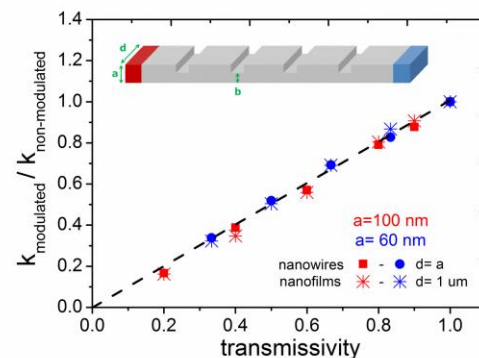


Figure 2. The thermal conductivity of two periodically modulated nanowires with $a = d$, and $a = 100$ nm (red squares) and $a=60$ nm (blue dots) versus the transmissivity. The length of the constriction is $c=10$ nm.

(dashed lines).

In Figure 1 it can be seen that the length dependence of the thermal conductivity is similar to that of the non-modulated nanowire for not very thin constrictions. It becomes though significantly steeper when a constriction becomes thin. Based on the steepness of the length dependence of the thermal conductivity, a transition between two regimes can be distinguished. This transition is clearly shown in the temperature profile across the modulated nanowire [12]. In non-very thin constrictions, e.g. 90 nm, the temperature profile is continuous and phonon transport is diffusive. When the constriction becomes thinner, e.g. 60 nm, a small discontinuity appears. This is the transition point. In thinner constrictions, e.g. 20 nm, the temperature profile is discontinuous. The discontinuity in the temperature profile is the signature of ballistic phonon transport across the constriction. A critical width can be identified below which phonon transport becomes ballistic. The ballistic transport is quantitatively described by a constriction thermal conductance K_C [12]. This ballistic conductance is analogous to the thermal contact conductance. It is determined by the width mismatch between the nanowire and the constriction, namely the constriction transmissivity $Tr = A_c/A_w$ where A_w and A_c respectively denote the cross sections of the wire and of the constriction. For the geometries of Figure 1, it holds: $Tr = b/a$, where a and b are respectively the widths of the nanowire and of the constriction. The constriction thermal conductance K_C scales with the transmissivity Tr according the relation:

$$K_C \propto (1-Tr)^{-1} \quad [12].$$

The analysis of the data showed that in this regime the effective thermal conductivity of the modulated nanowire can be decomposed into two contributions: (i) of the thermal conductivity of the non-modulated segments of the nanowire, and (ii) of the contribution of the constriction thermal conductance. The data can be interpreted by the approximate relation: $R_{mw}^{th} = R_C^{th} + R_w^{th}$, where R_{mw}^{th} , R_C^{th} , R_w^{th} are the thermal resistances of the modulated nanowire, of the constriction and of the non-modulated nanowires respectively. It holds that $K_C = 1/R_C$.

In the presence of multiple constrictions the thermal conductivity decreases more significantly than by a single constriction. For adequate modulation density, the decrease is proportional to the nanowire transmissivity [12]. This behavior is illustrated in Figure 2. In this regime, the thermal conductivity cannot be decomposed to distinct contributions and the signature of the single constriction thermal resistance is absent. The temperature profile across the nanowire has been found continuous. It can be thereby concluded that phonon transport is diffusive.

Let us now explore the transition from the ballistic constriction resistance behavior to the transmissivity behavior that takes place as the number of constrictions increases. We have performed simulations in nanowires with fixed length and with variable number of constrictions, i.e. variable modulation length as shown in the schematic representation in Figure 3. In Figure 4a it is shown the thermal conductivity of a modulated nanowire of fixed length versus the number of constrictions modulating its width. The different curves correspond to different constriction widths.



Figure 3. Schematic representation of a nanowire partially modulated by constrictions.

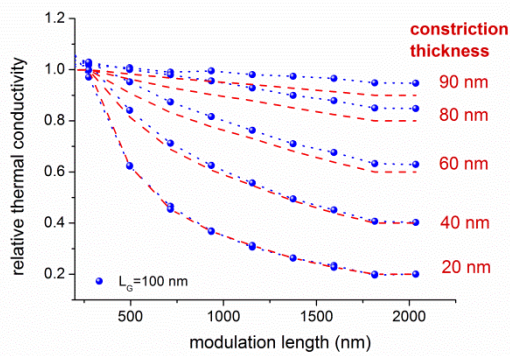


Figure 4a The thermal conductivity of the modulated nanowire relative to that of the non-modulated nanowire versus the modulation length for various constriction thicknesses. The red lines are the fittings of the phenomenological equation.

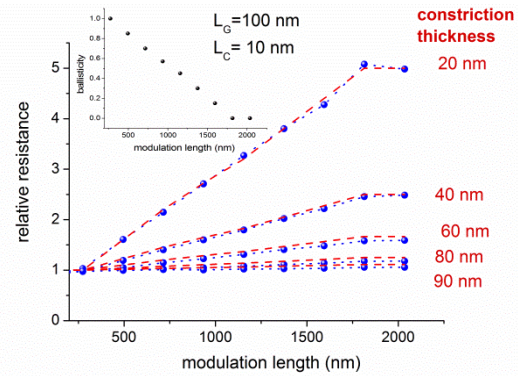


Figure 4b As in Figure 3a, for the relative resistance. The inset shows the fitting parameter χ versus the modulation length.

In Figure 4a, it can be seen that the thermal conductivity decreases gradually with a decreasing rate as the number of constrictions increases. It decreases more as more constrictions are added. This is because more constrictions provide more scatterers for phonons. In Figure 4b it is shown the resistance as a function of the number of constrictions. It can be seen that the resistance increases first linearly with the number of constrictions. The linear dependence implies that each time a constriction is added, a resistance proportional to R_c is added to the overall resistance. This holds until a certain resistance plateau is reached. At this plateau the thermal conductivity is proportional to the nanowire transmissivity. In this regime the thermal conductivity is independent of the number of constrictions. This behavior can be interpreted by the phenomenological equation:

$$R = R_w(L) \left[1 + (1 - \chi) (Tr^{-1} - 1) \right] + \chi N R_c$$

where $R_w(L)$ is the thermal resistance of the non-modulated segment of the nanowire with length L , N is the number of constriction and χ is the ballisticity of the nanowire. The parameter χ is a fitting parameter that is determined by the Monte Carlo simulations. It is plotted in the inset of Figure 4b. The data of this fitting plot were determined by the curve of Figure 4a for constriction thickness 20 nm. It has been found to successfully interpret all the curves shown in Figure 4. Parameter χ decreases nearly linearly up to the critical plateau. For $N=1$ it holds $\chi=1$ which corresponds to the single constriction ballistic regime. For $N > N_{\text{plateau}}$, $\chi \sim 0$ which corresponds to the scaling law with the transmissivity.

The calculated thermal conductivity and thermal resistance using the above phenomenological equation is shown in Figure 4 with red lines. It can be seen that the thermal resistance is interpreted extremely good by the above phenomenology. The thermal conductivity is also interpreted equally well for thin constrictions below the transition regime. Deviations have been found for not very thin constrictions. This is to be expected since above the critical thickness, the constriction thermal resistance R_c that is used in the phenomenological equation is not a well defined [nano]. The above equation indicates that when a small number of constrictions are present in the nanowire, they act as ballistic thermal resistances. As the number of constrictions increases, they gradually contribute more to the nanowire boundary scattering and to reduce the conduction of phonons through the modulated nanowire. For adequate number of constrictions the geometrical transmissivity of the structure determines the thermal conductivity.

3. Main conclusion

The thermal conductivity of width-modulated nanowires decreases gradually with increasing number of modulations. The decrease can be interpreted by the additional constriction thermal resistance with increasing number of constrictions. After a certain number of constrictions, the thermal conductivity depends on the transmissivity of the structure and not on the number of constrictions.

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