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Role of boundary roughness on heat transport in mesoscopic silicon ribbons at low temperatures

A. Ramiere[1], J. Amrit[1] and S. Volz[2]

[1] *Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur UPR CNRS 3251, Université Paris-Sud, Rue John von Neumann, F-91403 Orsay, France*

[2] *Energétique Moléculaire et Macroscopique, Combustion, UPR CNRS 288, Ecole Centrale Paris, Grande Voie des Vignes F-92295 Chatenay-Malabry, France*

We use Monte Carlo simulations based on phonon gas particles to study the role of the boundary roughness on the heat transport in silicon micro-ribbons at temperatures below 2K. The thermal conductivity and the energy transmission coefficient are calculated for different surface roughness. In the diffusive (Casimir) limit we find the T^3 behavior of the thermal conductivity as predicted by the Debye model. We report deviations of this comportment for very low temperatures and for smooth surfaces. The energy transmission is almost unity up to a cut-off frequency, which is correlated to the roughness. These observations are interpreted by a change in the scattering regime of the phonons at the surface boundaries shifting from specular to diffuse, depending on the root mean square roughness σ_{rms} and the dominant phonon wavelength λ_{dom}.

I. INTRODUCTION

Silicon nanowires have strong potential for thermoelectric applications[1]. The efficiency of these devices requires an enhanced figure of merit ZT [2], which can be controlled by the thermal conductivity. The role of surface roughness on the thermal conductance becomes predominant, especially at low temperatures. Intensive studies, experimental as well as numerical, have been carried out to determine the thermal conductivity of silicon nanowires for temperatures above 20K [3–5]. The main difficulty is to quantitatively identify the different contributions to the scattering processes taking place in the nanowire. And the impact of the boundaries roughness is overwhelmed by phonon-phonon normal and Umklapp processes, impurities, etc… On the other hand, at very low temperatures, the characteristic time of interactions for three phonon processes becomes very large compared to the other scattering processes and they can be neglected according to Matthiessen's rule [6]. Today, we are able to fabricate nanowires almost free of imperfections and therefore boundary scattering becomes the main heat transport channel at very low temperatures.

Our system is a mesoscopic silicon ribbon of 4µm long, 1µm in width and one unit cell in thickness. It can also be seen as a quasi 2D microwire. The mean free path is much greater than the width of the sample so that the ballistic regime is well established. Also, the dominant wavelength is smaller than the width. Consequently, phonon confinement effects are neglected and we thus treat phonons as classical particles.

II. SIMULATION MODEL

The Monte Carlo method adopted here is similar to the approach used by the Peterson [7]. The advantage of the low temperature limit is that an analytical expression for the energy integral is avalaible. Indeed, when integrating over the frequencies the energy distribution given by:

$$B(\omega)=\frac{3\hbar}{2\pi^2 c_D^3}\frac{\omega^3}{e^{\beta\hbar\omega}-1} \tag{1}$$

becomes non-existent above he Debye frequency ω_D. The upper limit is hence extended to infinity.

$$\varepsilon=\int_0^{\omega_D}B(\omega)d\omega=\frac{\pi^2 k_B^4}{10c_D^3\hbar^3}T^4 \tag{2}$$

where c_D is the Debye sound velocity.

Contrary to previous Monte Carlo models [7], [8], we calculate the total number of phonons by summing the energies associated with each phonon until the energy given by eq.2 is reached.

A phonon frequency, which is randomly selected in the energy distribution, defines the phonon wavelength λ. The phonon is then launched at the entrance of the ribbon and it ballistically moves until it encounters a boundary. The collision between the phonon and the boundary is elastic because the system is in vacuum and radiations are negligible. The reflected phonon is assigned with an angle θ_S, which is randomly picked in a normal distribution centered on the incident angle θ_i. The FWHM of this distribution is related to the probability for the phonon to be specularly scattered as calculated by Ziman [9] and is given by:

$$p(\sigma_{rms},\lambda)=\exp\left(-\frac{16\pi^3\sigma_{rms}^2}{\lambda^2}\right) \tag{3}$$

The phonon undergoes scattering until it is either reflected back to the entrance and is counted as a loss, or it goes across the ribbon and is counted as transmitted.

III. RESULTS AND DISCUSSIONS

The frequency dependant energy transmission coefficient is statistically determined and is given by $\tau_\varepsilon(\omega)=N_{in}/N_{out}$ where N_{in} is the total number of phonons of frequency ω and N_{out} is the number of transmitted phonons at the same frequency. The results are shown in Figure 1 for boundaries of different roughnesses. We observe that at low frequencies, the transmission is unity and decreases abruptly around a cut-off frequency to reach a limit of 0.35. The deviation from $\tau_\varepsilon=1$ occurs at lower frequencies as the surface roughness is increased. In other words, as the surface roughness increases the cut-off frequency decreases.

The thermal conductance is calculated from the heat flux Q input in the ribbon and the temperature difference ΔT between the two extremities of the wire. Taking unity for the energy transmission, the heat flux along the length of the ribbon is given by [10]:

$$Q = \frac{S_R}{V_{res}} \sum_i \hbar \omega_i c_D \cos\theta_i \qquad (4)$$

Where S_R and V_{res} are respectively the cross-section of the wire and the volume of the heat bath.

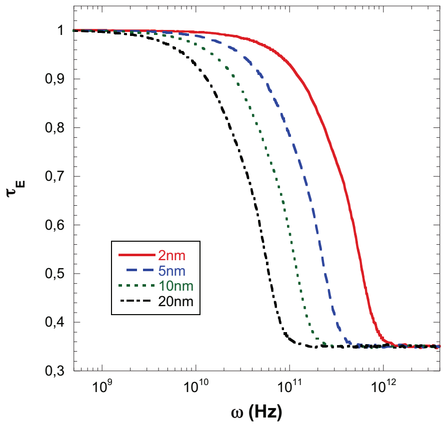

Fig. 1. Energy transmission versus frequency for roughnesses ranging from 2nm to 20nm.

Using the total energy of phonons going through the ribbon, as given by eq.2, we obtain the temperature at the cold extremity and therefore ΔT. The thermal conductance is then simply given by $\kappa = Q / \Delta T$.

In Figure 2, the results show that the thermal conductance is proportional to T^3 for high temperatures and/or high roughnesses as expected for the Casimir regime. The thermal conductance decreases with higher surface roughness. At temperatures below 1K we see deviations from the T^3 law, which becomes more pronounced for smoother surfaces. In Figure 2 we also compare our simulations to the experimental results of Heron *et al.*[11]. Their thermal conductance measurements were performed by using the 3 ω technique on a silicon nanowire of length 10 µm and of cross-section 200 x 100 nm^2. It is interesting to notice that the orders of magnitude are very similar and we have the same behavior below 1K.

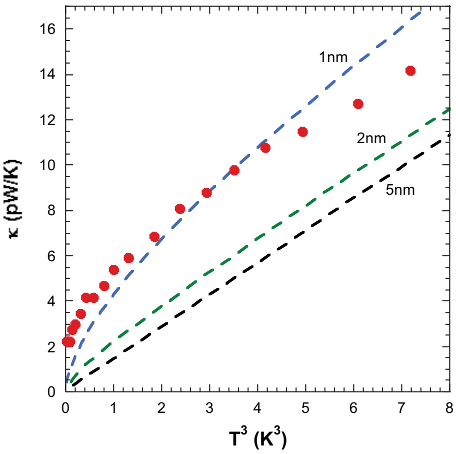

Fig. 2. Thermal conductance with temperature. Dashed lines for different roughnesses of 1nm, 2nm and 5nm. Full circles depicting the experimental results by Heron *et al.*[11].

We explain this behavior by the transition from specular to diffusive scattering at the boundaries. With increasing temperatures, $p(\sigma_{rms}, \lambda)$, given by eq.3, decreases rapidly. Taking $p = 0.1$ as a criterion for the onset of the diffusive regime provides the ratio $\sigma_{rms} / \lambda = 7\%$. Below this latter value, the effects of specularity are significant. This explains the observed trends.

IV. CONCLUSION

Based on first principles, the role of the boundary surface scattering on the thermal conductance of a mesoscopic ribbon structure (4µm in length, 1µm in width) is examined by using a Monte Carlo approach.

The simulations are done at very low temperatures where the ballistic regime occurs and where phonon-surface roughness interaction is predominant. The diffusive T^3 behavior of the thermal conductance is correctly produced in the simulations.

Our results show a deviation from this law when the specular regime appears for $(\sigma_{rms} / \lambda) < 7\%$. Finally, we note that our simulation method maybe be relevant to study the impact of geometry of the ribbon on the thermal conductivity in the ballistic regime.

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