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Surface effect on the phonon transport of silicon nanowire

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Abstract. Thermal conductance measurements are presented on nanostructured individual single crystalline Si suspended nanowires at low temperature. The mechanically suspended silicon nanowires with different sizes (130nm by 100nm and 130 nm by 200nm) are fabricated by e-beam lithography from Silicon On Insulator (SOI) substrate. The thermal conductance of the ballistic phonon wave guides is measured by means of an ac technique, the 3 ω method, using a niobium nitride transducer deposited on top. The geometry of the nanowire is chosen to match the order of magnitude of the dominant phonon wave length in silicon at low temperature which is of the order of 100 nm at 1K. A regular cubic law is observed at high temperature, but a deviation is measured at the lowest temperature with a saturation of thermal conductance which is attributed to the reduced geometry of the nanowire. The experimental results are in agreement with the Casimir theory taking into account the surface state (roughness) of the silicon wire. The deviation observed at low temperature is a clear signature of the consequence of the low dimentionality of the wire as well as the surface effects on the phonon transport.

1. Introduction

The understanding of heat transfert at the nanometer length scale is one of the most difficult scientific challenge of the present decade. The fabrication of nanomaterials (nanowire nanoparticles etc..) are now wide spread and hence their thermal properties are a large subject of experimental studies [1]. Most of the experiments are made at room temperature and more specifically thermal conductance of semiconductor nanowires or carbon nanotubes have been widely probe [2, 3, 4, 5]. At low dimension specific thermal behaviours are expected due to the importance taken by the surfaces in the phonon scattering processes [6] like high thermal conductance in defectless carbon nanotubes or deviation from the bulk in semiconductor nanowire thermal conductivity due to the reduced size. Since few years many experimental results have been obtained [1] due essentially to the progresses in measurement method. However, the thermal properties at low temperature remain largely unexplored [7, 8] despite numerous interesting phenomena predicted theoretically [9]. We present thermal conductance measurement performed on suspended silicon nanowires at low temperature. In our experiment the dimension of the sample is of the same order of magnitude as the dominant phonon wave length λ_D at low temperature; this may have dramatic effects on the amplitude of the thermal conductance. We show that the thermal conductance of the nanowires follows a regular T^3 law at high temperature but deviations are observed for the lower temperatures which is explained by the reduced dimensions of the phonon conductors.

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2. Experimental details

The small dimension imposes the development and fabrication of new devices and experimental set-up to measure in good conditions the thermal properties. Also the instrumental method has to be adapted to the small size of the sample implying many constraints on the connection of the sample or due to the amplitude of signal to noise ratio. Moreover the temperature has to be controlled at the nanometer length scale which can be very challenging in the case of self suspended nanostructures.

We study in this work the thermal conductance of suspended silicon nanowire using the 3ω method. The nanowires have a cross section around 100nm. The 3ω method is perfectly adapted to the measurement of thermal properties of nanowires (see [10, 8, 5]). The suspended wires are fabricated in the CEA-LETI facilities from Silicon On Insulator (SOI) 200 mm substrate (see the schematic given in Fig. 1 and 2). A first step of thermal oxidation and buffered HF etching is used to thin the upper layer down to 130 nm. The wire and the pads are then written on negative resist (Shipley UVN2) using e-beam lithography. The pads and the wire are structured in the upper silicon layer by Reactive Ion Etching down to the SiO₂ layer. The SiO₂ layer is then removed with buffered HF. The under-etching liberates the Si wire which remains suspended between the two pads. The pads are electrically isolated from the crystalline silicon underneath thanks to the SiO₂ layer. Si nanowires with large aspect ratio were obtained with lengths of 5 to 15 μ m and cross sections of 130 by 200 nm or 130 by 100 nm.



Figure 1. Fabrication process of silicon nanowires from silicon on insulator substrate. Step 1) corresponds to the thinning of the silicon layer down to 130 or 100 nm, step 2) describes the ebeam lithography of the nanowire on the Shipley resist, step 3) shows the etching of the silicon layer by RIE process and finally the step 4) corresponds to the etching of the SiO₂ underlayer by the buffered HF.



Figure 2. SEM view of a suspended silicon nanowire and schematic of the device composed by the transducer and the silicon nanowire.

Following these fabrication steps, a transducer is deposited onto the surface of the pads and the wire. A niobium nitride (NbN) thin films transducer is directly AC sputtered onto the surface of the device (pads and nanowire, see Fig. 1). This thermometric element undergoes a metal to insulator transition at low temperature, and hence exhibits a large temperature coefficient of resistance $\alpha = 1/R(T) \times dR(T)/dT$, on the order of $\alpha = 0.3$ K⁻¹ at 1K.

By working at sufficiently low frequency, we can consider that the signal is only dependent on the thermal conductance of the nanowire. In that limit, called quasi-static limit, the thermal

conductance and the voltage at 3f is related through the formula:

$$V_{3\omega} = \frac{4R^2 I_{ac}^3 \alpha}{\pi^4 K} \tag{1}$$

where K is the thermal conductance R the resistance of the transducer, I_{ac} the rms applied current and α the coefficient of temperature. The system is actually constituted by the silicon nanowire and on top of it the transducer. The silicon wire has to be indeed the principal thermal conductor. Therefore, one has to make sure that no major heat loss appears through the transducer as a parallel thermal path. The geometry of the wire imposes an electrical resistance for the transducer varying from 50 to 100 kOhm between 0.5 and 4 K. We then evaluate the expected thermal conductance of the transducer through the Wiedemann-Franz law (KR/T = constant) valid for amorphous materials at low temperature, where the thermal conductance is dominated by the transport of heat by the electrons. Using this relation, we calculated the thermal conductance expected for the transducer on the order of 10^{-13} W/K in the better case, which is two orders of magnitude smaller than that expected for silicon (10^{-11} W/K at 1K) over the entire temperature range of our measurements.

3. Thermal conductance

The temperature variation of the thermal conductance of a 5 μ m long (section 130 by 200 nm) nanowire is shown on the Fig. 3 and on the Fig. 4 the temperature variation measured on a 7 μ m long (section 130 by 100nm). In the inset of the Fig. 3 and Fig. 4, K(pW/K) is plotted versus T^3 to highlight the regular cubic power law behaviour of the thermal conductance. At low temperature the phonon transport in single crystalline silicon is ballistic; the phonon mean free path is only limited by the geometry of the wire. Hence the phonon transport is governed by the boundary scattering on the rough surfaces of the wires; this limit is known as the Casimir regime.





Figure 3. Thermal conductance versus temperature for the $130 \times 200 \text{ nm}^2$ silicon nanowire.

Figure 4. Thermal conductance versus temperature for the $130 \times 100 \text{ nm}^2$ silicon nanowire.

So as a first conclusion, at sufficiently high temperature, as expected we recover a regular cubic power law for the thermal conductance. However as the temperature is lowered a deviation from the T^3 law is observed as reported in reference 8. In the first case (the bigger nanowire), only a slight deviation is evidenced at lower temperature, below 0.7K. But in the second case the

deviation is much more pronounced with a saturation arising below 3K. As it is expected from existing theories and experiments [7, 9], the low temperature limit of the thermal conductivity can be strongly perturbed when the sizes of the structures are at the nanoscale.

The thermal conductance of a conductor with a section of the order of the dominant phonon wave length $\lambda_D = \hbar v_s/2.82k_BT$ (v_s is the sound velocity) can saturate to one quantum of thermal conductance per phonon quantum channel as the temperature is lowered given by:

$$K_Q = \frac{\pi^2 k_B^2 T}{3h} \tag{2}$$

Because in a rectangular shape wave-guide only four phonon polarizations are expected, then only four thermal quantum channels exist in each direction of the heat flow in our system; that is why we have normalized the measured thermal conductance to $8K_Q$ in the Fig. 3 and Fig. 4. In silicon, λ_D is of the order of 100nm at 1K, so the observed saturation of the thermal conductance to the universal value cannot be explained by the reduced section of the nanowire; this stauration is expected at much lower temperature. As observed in these samples a saturation to the universal thermal conductance may arise from an other origin than the quantification of the thermal conductance per conducting channel. At low temperature due to the increase of λ_D and hence the increase the phonon mean free path, the phonon transport may be dominated by specular reflections and hence increase the thermal conductance as compared to the value given by the Casimir theory where the thermal transport is dominated by the boundary scattering on the rough surfaces. Finally, we cannot exclude that if the phonon transport becomes highly specular then the hypothesis of a well defined temperature all along the wire made in the 3ω method is wrong. In that situation, the equation 1 would be no anymore valid. This might also explain the observed discrepancy between K(T) and the regular cubic law.

4. Conclusions

To conclude, we have shown that the 3ω method is well suited for the measurement of small thermal signal on suspended structures. Accurate value for the thermal conductance is found for silicon at low temperature which can be of great importance for the future application in calorimetric measurement. The deviation from the Casimir model can be explained by the increase of the mean free path of the phonon which leads to an increase in the thermal transport, a clear signature of the surface effects at the nanoscale.

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