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Thermal resistance at constrictions in 2D mesoscopic ribbons at low temperatures

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Abstract. Phonon transport in junctions formed between suspended membranes of the same material is studied using Monte Carlo method. The investigation is conducted at 1K for systematically chosen ratios of (d/D) where d is the junction width and D the membrane length. The influence of surface roughness is taken into account. The dependency of the constriction thermal resistance (in $\mu\text{mK/W}$) is established: $R_J \approx [2.4 + 2.0 \times (d/D)^{-1/2}] \times 10^9$. The average and frequency dependent transmission coefficients are determined as a function of (d/D) . These structural configurations are inherent in thermoelectric; and graphene and silicene related applications.

1. Introduction

In this paper phonon transport in a uniform material composed of two rigid suspended mesoscopic membranes connected with an abrupt junction/bridge is studied at low temperatures (see figure 1). In particular we show the apparition of a thermal boundary resistance R_J at the membrane/junction interface. The latter is due to the mismatching of vibrational modes because of the sharp change in the geometry. The junction diameter d and the root mean square surface roughness σ of the structure are also taken into account. We recall that thermal characterization of these structural configurations are vital for thermoelectric; and graphene and silicene related nanotechnology applications at room temperatures.

2. Sample set-up and Monte Carlo technique

Our study is conducted on a 2D material with a surface roughness of 2.4 nm. The membranes are $100 \times 100 \mu\text{m}$ squares and the junction length is fixed to $10 \mu\text{m}$. The junction diameter is varied from $1 \mu\text{m}$ to $10 \mu\text{m}$. The sample is divided into cells of constant length $\Delta = 0.5 \mu\text{m}$. Our approach in implementing the Monte Carlo method is similar to that of Peterson¹ and to that described in ref. [2]. Phonons (of different polarizations L or T and frequencies) are randomly selected in a Planck-like distribution to populate the hot membrane until the total energy corresponding to the set temperature of the membrane is attained. Flexural modes, which are fully diffusely scattered, are neglected as the main objective is to highlight the geometrical dependencies of R_J . The trajectories of the phonons (defined by randomly chosen angles) are ballistic and the nature of the boundary scattering at the walls is determined by the specularity factor $p(\sigma, \lambda) = \exp(-16\pi^2 \cos(\theta) \sigma^2 / \lambda^2)$ where θ is the angle



between the phonon wave vector and the normal to the ideal smooth surface. Under the physical conditions of this simulation, phonon-phonon and Umklapp processes are inoperative.

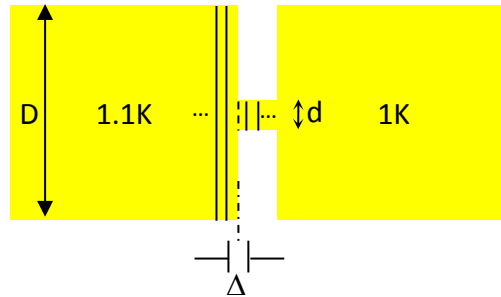


Figure 1. Junction/Bridge of width d between two suspended membranes of sides D . The abrupt form is chosen to enhance the effect of the junction/membrane thermal resistance. The latter is determined over the length Δ , defined in text.

3. Thermal resistance and transmission coefficients at membrane-junction interface

The thermal conductance h_J at the junction/membrane interface is defined as: $h_J = (Q^+ - Q^-) / \Delta T$ where Q^+ and Q^- are respectively the energy associated with the phonon flux leaving and entering the membrane to and from the junction, and ΔT is the temperature jump over the cell length Δ at the interface. The junction/membrane thermal boundary resistance is now defined as: $R_J = d / h_J$. In figure 2, R_J is plotted as a function of $(d/D)^{-1/2}$ to highlight the following linear behaviour in $\mu\text{m.K/W}$: $R_J \approx [2.4 + 2.0 \times (d/D)^{-1/2}] \times 10^9$. The numerical coefficient is simply the thermal resistance due to the conductance over Δ .

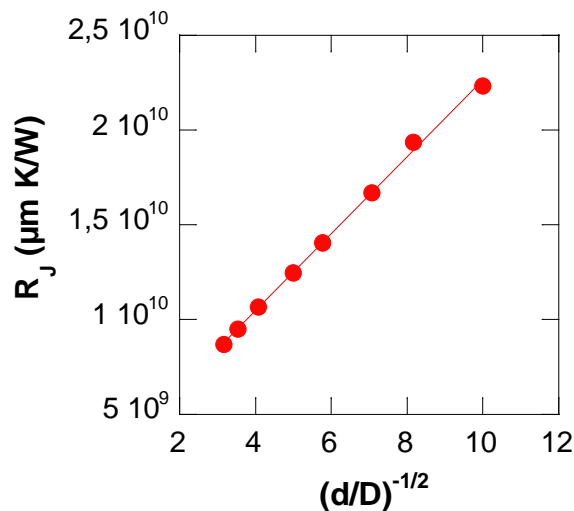


Figure 2 Thermal resistance at membrane/junction interface in Silicene material.

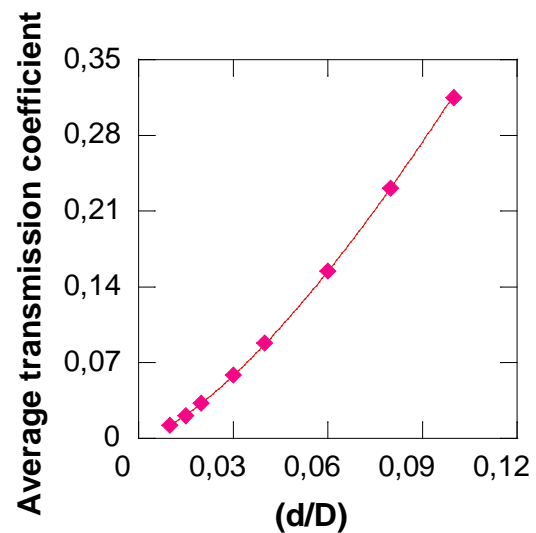


Figure 3. Power law evolution of the average transmission coefficient as a function of (d/D) .

The average transmission $\bar{\tau}$ is determined using the definition³ $h_J = (1/4)C_2\nu_D\bar{\tau}$ where the specific heat $C_2 = (\partial E_{2D} / \partial T)$, with E_{2D} being the 2D energy, and ν_D is the Debye velocity defined as $\nu_D^{-2} = \sum_i (1/\nu_i^2)$, with $i = L, T$. All numerical values used are that of Silicene material⁵. Figure 3 shows that $\bar{\tau}$ follows a power law with (d/D) given by: $\bar{\tau} = 8.23(d/D)^{\sqrt{2}}$. The frequency dependant transmission for each polarisation entering the junction undergoes a change as a function of the junction width as shown in figure 4 (a) and (b). Also, the transmission of L modes dominates over that of T modes.

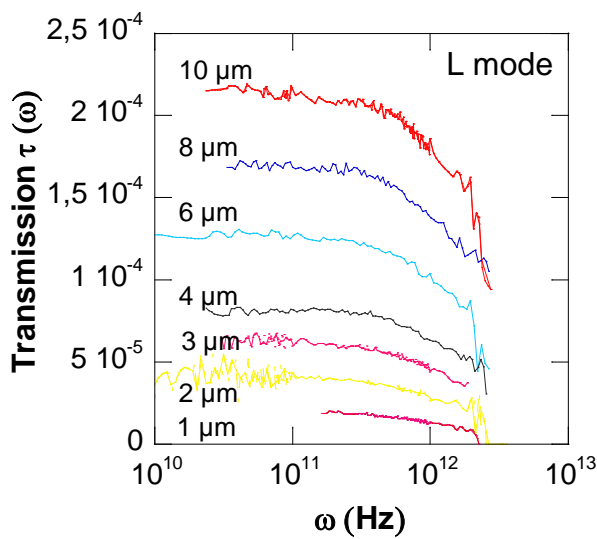


Figure 4a. Transmission of mode L membrane/junction interface.

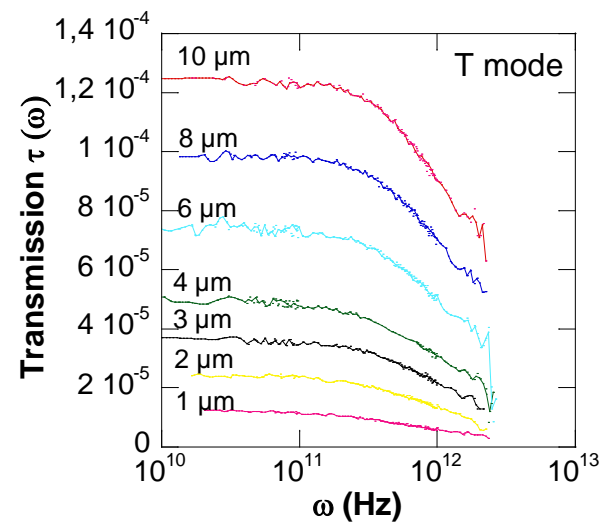


Figure 4b. Transmission of mode T at membrane/junction interface.

Finally, we note that an analytical solution of the thermal transport in this 2D configuration is discussed by Cross and Lifshitz⁴. The novelty in our study is that we have taken into account the surface roughness. Details of our full study shall be given in ref. [5] in preparation.

Conclusions

Using the Monte Carlo method at $\sim 1K$, we have demonstrated that the thermal resistance at the membrane/bridge interface varies as $(d/D)^{-1/2}$. The average transmission coefficient $\bar{\tau} \propto (d/D)^{\sqrt{2}}$. The transmission coefficient of modes L and T are independent of frequency for small ω , but it varies with the junction width d .

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