Phonon Multiplexing Through 1D Chains and Phonon Flow Through 1D Channels and Nanospheres

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Phonon propagation through atomic structures has become an important study issue. The most important application arises in the thermal field, since phonons can carry thermal and acoustic energy. The technological advantage makes it possible to engineer at nanoscale thermal and acoustic paths as desired. In this work, we present two cases, the engineering of 1D phonon filters and the phonon flow through 1D channel and nanospheres.

1. 1D phonon filters

A linear numerical method was developed in order to analyze the scattering and filtering of phonons in 1D atomic structure. Only transverse propagation modes were taken into account. Bonding forces between the atoms were assumed to be linear; also these forces were restricted to be first nearest neighbour interaction.

A simple phonon multiplexer proposed by Dobrzynski [1] was analyzed. It consists of two mono-atomic chains of atoms and a coupling structure between them, which is made out of two atoms connected together. Dobrzynski´s results [1] were verified making it possible to use the developed model in further analysis. Earlier analysis of the structure did not establish a way of changing the wave length in which the phonon transfer occurs. Taking advantage on the friendly numerical methods, it was possible to establish simple rules that enable us to actually select a wavelength of transmission and tune the structure by changing its constitutive parameters such as atoms masses and bonding forces. The multiplexer efficiency was also studied, setting the limits of well performance of the filter. Finally, the frequency analysis led us to obtain the energy gaps between the propagating modes. The developed method allows studying more complex structures than the one presented here. In summary, we find how the parameters of the structure allow us design phonon filters.

2. Phonon flow 1D channels and nanospheres

Studies on phonon propagation through nano channels and nanospheres are expected to allow the exploration of thermal transport at 1D and 0D zero regimes. Recently, 1D channel thermal properties have been studied as a consequence of the advance fabrication techniques [2]. The studies have shown that although electrons and phonons obey completely different statistics, however, in 1D wire and at low temperatures they transport the same amount of thermal energy [3]. Deviations from the exact thermal quantization have been reported as functions of the wire geometry and wire coupling to the interfaces [3][4]. Estimations of the thermal conductivity have been carried out following Landauer formalism in which the thermal conductance of 1D channel is given as a function of the transmission coefficient [3].

In this work, the transmission coefficient is studied as a function of the variation of transversal area dimensions along the thermal conductor (i.e. 1D channel and 400nm diameter sphere) and at their interfaces. Only longitudinal modes are considered in the phonon propagation modeling. These results show peaks associated with the phonon trapping and phonon transmission and depend on:

- The relation of the minimum channel and the contact area at the interface;
- The channel length; and
- The propagating phonon wavelength.

Although, analytical methods could give more accurate results when the channel structure becomes too complex, they may not be solvable. Thus, numerical methods became necessary to obtain the transmission coefficients through channels. Two methods, the Frobenius and the Finite Differences, were implemented. Early results showed important issues in both convergence and computing time, so there is trade off.

Frobenius method takes less computing time, but at smaller wavelengths it loses its convergence. On other hand, Finite Differences method gives

more accurate results at higher wave vectors, but the discretization required has to be high in order to obtain small errors. Initial results were obtained using simple channel structures so that the numerical results can be compared with analytical results [3]. We found that the transmission coefficients obtained are very sensitive to the numerical method implemented. It is therefore extremely important to use a high number of points or coefficients independent of method that is being used in order to obtain good approximations. Nevertheless, it was found that the Finite Differences method is more reliable than Frobenius method because its results do not depend on expansion series convergence radius.

References

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