Physica E 88 (2017) 97–103

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Ballistic phonon thermal transport across topologically structured nanojunctions on Gold wires

M. Belhadi[a,*], A. Khater[b]

[a] Département des Sciences de la Matière, Institut des Sciences et de la Technologie, Centre Universitaire de Tamanghasset, BP10034 Sersouf, Tamanghasset, Algeria

[b] Laboratoire de Physique de l'Etat Condensé UMR 6087, Université du Maine, 72085 Le Mans, France

ARTICLE INFO

Keywords:
Heat conduction
Phonon states and bands, normal modes and phonon dispersion
Quantum wires
Ballistic transport

ABSTRACT

We investigate the coherent phonon thermal transport at low temperatures in Gold nanowires, in order to study the effects of scattering on the lattice thermal conductivity. Three types of shaped joint nanostructures are employed in our calculation. We present a detailed study of the thermal conductance as a function of the temperature for different shaped joint. This is done by solving the phonon Boltzmann transport equation in the ballistic regime and calculating the transmission rates of the vibration modes through the consideration of the phonon group velocity modification in the system. The transmission properties are calculated by use of the matching method in the harmonic approximation with nearest and next nearest neighbor force constants. The results show that the transmission probabilities depend on the type of joint nanostructure. The pronounced fluctuations of the transmission spectra as a function of the frequency can be understood as Fano resonances. It is also found that the behavior of the thermal conductance versus temperature is qualitatively different for different nanostructures and depends sensitively on the width of the shaped joint.

1. Introduction

Nanometer scale material forms exotic structures and are attracting a great interest due to the novel physical and chemical properties that appears in these materials. Interest in nanostructures is motivated by the increasing need to acquire knowledge of their properties for high technology applications. There is, consequently, an increasing volume of experimental data to elucidate the structural [1], magnetic [2], and electronic [3], properties of quasi-one dimensional nanostructures. Shaped joint in these materials at nanoscales may break the translation symmetry, which leads to several effects, such as localized states, wave reflection, and resonant scattering, [4].

Modern technology has enabled the fabrication of materials with characteristic dimensions of a few nanometers. Examples are superlattices [5], nanowires [6], and quantum dots [7]. The ability to generate such one-dimensional nanostructures is essential to modern science and technology [8]. It is generally accepted that quantum confinement of the electrons in low dimensional systems may provide one of the most powerful means to control the properties of functional materials. Among these materials, one dimensional nanostructure such as wires has become the focus of an intensive research owing to their unique properties.

Metallic nanowires, have attracted a great deal of attention, since they show very interesting properties from a basic science viewpoint, as well as great potential in applied fields such as nanoelectronics, [9]. This interest has mainly risen with the fact that very thin metal nanowires were shown to be stable structures [10]. The atomic gold nanowire is the best-studied atomic-sized conductor, and a great deal of detailed information is available from experiments [11] and theoretical studies [12]. A wealth of experimental and theoretical studies on ballistic electron transport in various configurations has been reported [13]. In contrast, little attention has been paid to the study of heat transport by phonon in nanostructures. Recent theoretical, and experimental findings, proved the existence of a quantum of thermal conductance in ballistic regime, which is similar to a quantum of electronic conductance.

In recent years, phonons thermal transport was reported in several of nanostructures. Using the Landauer formulation of transport theory, the thermal conductance in dielectric quantum wire at low temperatures was calculated [14], and verified by experiment [15]. Motivated by these experimental and theoretical works, phonon thermal transport were investigated in various quantum wire structures such as a nanowire with surface roughness [16], with typical structure defect [17], and with stub quantum structures [18], in an asymmetric

* Corresponding author.
E-mail address: mbelhadi@yahoo.com (M. Belhadi).

http://dx.doi.org/10.1016/j.physe.2016.12.009
Received 18 April 2016; Received in revised form 15 November 2016; Accepted 23 December 2016
Available online 24 December 2016
1386-9477/

quantum structure [19], and four-terminal mesoscopic dielectric system [20]. In recent work we have calculated the phonon transmission coefficient in quasi-1D systems [21], by applying formalism for the vibration dynamics and scattering comparable to that of Landauer-Büttiker.

This paper is aimed to develop a theoretical modeling to investigate the effect of shaped joint nanostructure on heat transport in Gold nanowires. This is done by calculating the transmission rates of the vibration modes through the consideration of the phonon group velocity modification in the system. Our challenge is to calculate the phonon transmission probabilities for the individual phonon modes, as a function of the propagating frequencies of the system and to determine the heat transport by use of the Landauer-Büttiker formalism for thermal transport in the ballistic regime.

The paper is organized as follows. In Section 2, we present the phonon heat transport formalism. Section 3, review the dynamical properties of the perfect Gold nanowire. A description of the formalism for calculating the phonon transmission via a shaped joint nanostructure is described in Section 4. The transmission spectra are calculated by use of the matching method in the harmonic approximation with central nearest and next nearest neighbor force constants. The salient numerical results are presented in Section 5, along with the conclusion of the paper.

2. Phonon heat transport formalism

Landauer formulation of quantum transport showed that when elastic scattering dominates, the electrical conductance can be related to the transmission coefficient of the electron waves [22]. The application of similar ideas to the phonon counterpart was recently derived by a number of authors [23].

Let us imagine a perfectly harmonic and translational invariant system, totally free of defects. In this situation, the heat transfer associated with a small temperature difference, is given by the sum of the contributions of the individual phonons. If we look at the transport by the left moving phonons, the heat flow is given by

$$\mathbf{Q_{LR}} = \sum_{\nu} \frac{1}{(2\pi)^3} \int \mathbf{d^3k}\, \mathbf{v_{g\nu}}(\mathbf{q})\hbar\boldsymbol{\omega}_{\nu}\mathbf{n}(\mathbf{T_L}, \boldsymbol{\omega}_{\nu}(\mathbf{q})) \tag{1}$$

For the transport by the right moving phonons, the heat flow is given by

$$\mathbf{Q_{RL}} = \sum_{\nu} \frac{1}{(2\pi)^3} \int \mathbf{d^3k}\, \mathbf{v_{g\nu}}(\mathbf{q})\hbar\boldsymbol{\omega}_{\nu}\mathbf{n}(\mathbf{T_R}, \boldsymbol{\omega}_{\nu}(\mathbf{q})) \tag{2}$$

The phonon heat flow associated with a small temperature difference ΔT, is given by

$$Q = \Delta T \sum_{\nu} \frac{1}{(2\pi)^3} \int d^3q\; v_{g\nu}(q)\hbar\omega_{\nu}(q) \frac{\partial n(T, \omega_{\nu}(q))}{\partial T} \tag{3}$$

where q is the wave vector, $\omega_{\nu}(q)$ is the dispersion relation of the νth discrete mode, and $v_{g\nu}=d\omega_{\nu}/dq$ is the group velocity. T is the temperature, $\hbar$ is the reduced Planck's constant, $n(T, \omega_{\nu}) = [\exp(\frac{\hbar\omega_{\nu}}{k_B T} - 1)]^{-1}$ is the Bose-Einstein distribution function of the phonons and k_B is Boltzmann's constant.

The phonon thermal conductance κ is obtained from Q , which is the difference between Q_{LR} and Q_{RL}. $k=Q/\Delta T$ in the limit ΔT 0. Hence, at $T=(T_L+T_R)$ /2, the expression of thermal conductivity k can be written as [29]

$$k = \sum_{\nu} \frac{1}{(2\pi)^3} \int d^3q\; v_{g\nu}(q)\hbar\omega_{\nu}(q) \frac{\partial n(T, \omega_{\nu}(q))}{\partial T} \tag{4}$$

Finally, introducing the scaled variable $\beta=1/k_BT$, $\varphi_{\alpha}=aq_{\alpha}$ (α=x, y), $\Omega_{\nu}=\omega_{\nu}/\omega_0$ and $v_{g\nu}=d\Omega_{\nu}(q)/d\varphi_x$, gives the expression of thermal conductivity as:

$$\boldsymbol{k} = [\boldsymbol{\beta}\hbar\boldsymbol{\omega}_0]^2\boldsymbol{k_B}\boldsymbol{\omega}_0 \sum_{\nu} \frac{1}{(2\boldsymbol{\pi})^3} \int \mathbf{d^3q}\, \boldsymbol{\Omega}_{\nu}^2(\mathbf{q}) \frac{\partial\boldsymbol{\Omega}_{\nu}}{\partial\boldsymbol{\varphi}_x} \frac{\mathbf{e}^{\boldsymbol{\beta}\hbar\boldsymbol{\omega}_0\boldsymbol{\Omega}_{\nu}}}{(\mathbf{e}^{\boldsymbol{\beta}\hbar\boldsymbol{\omega}_0\boldsymbol{\Omega}_{\nu}} - 1)^2} \tag{5}$$

More generally we cannot assume a crystal totally free of defects, in our cases, the shaped joint introduce scattering at the boundaries. This can be taken into account, following the Landauer approach, through a transmission coefficient for energy transported across the nanostructure and we would find a thermal conductance as

$$k=[\beta\hbar\omega_0]^2 k_B\omega_0 \sum_{\nu} \frac{1}{(2\pi)^3} \int d^3q t_{\nu}(\Omega_{\nu})\Omega_{\nu}^2(q) \frac{\partial\Omega_{\nu}}{\partial\varphi_x} \frac{e^{\beta\hbar\omega_0\Omega_{\nu}}}{(e^{\beta\hbar\omega_0\Omega_{\nu}} - 1)^2} \tag{6}$$

where $t_{\nu}(\Omega)$ is the energy transmission coefficient from mode ν of left domain at frequency Ω across the shaped joint nanostructure into the modes of right domain. The effect of scattering is introduced through the transmission coefficient $t_{\nu}(\Omega)$, where $t_{\nu}(\Omega)$ can be derived by use of the matching method as we shall see in Section 4.

3. Phonon dispersion and group velocities

It is well known that phonon spectrum undergoes strong modification in nanostructures. It is particularly pronounced when the nanostructure dimensions are much smaller than the phonon mean-free path. It has been predicted [24] that the modification of phonon spectrum, in nanowires can lead to a significant decrease of the lattice thermal conductivity due to changes in the phonon group velocity and phonon relaxation rates [24,25]. The decrease of the phonon group velocity in nanostructures results in strong enhancement of the phonon scattering on defects [24].

The linearized equation of motion governing the fluctuation field for atoms located at sites l far from the shaped joint boundary in gold nanowire, is given in the harmonic approximation, by the following expressions

$$\omega^2 m(l)u_{\alpha}(l) = -\Sigma_{l'\neq l}\Sigma_{\beta}k(l, l')d_{\alpha}.\; d_{\beta}/d^2[u_{\beta}(l)-u_{\beta}(l')], \tag{7}$$

where (α, β) ∈{x, y}, m≡m (l) denotes the monatomic mass throughout the system, and $u_{\alpha}(l)$ represents the vibration displacement along the α direction. The radius vector **d** between atomic sites l and l', has Cartesian components d_{α} and $d=|\mathbf{d}|$. The force constants $k(l, l')$ between two sites are k_1 and k_2 for nearest and next nearest neighbors respectively. The system of linear equations from Eq. (7), may be cast in the form

$$[\Omega^2 I - D(z, \gamma)]|U> = 0. \tag{8}$$

$|U>$ is the displacement eigenvector in a unit cell. D(z, γ), is the dynamic matrix where $z=\exp(iaq_x)$ is a generic phase factor between neighboring sites, and I is the unit matrix. Note that $\Omega=\omega/\omega_0$ is a dimensionless frequency, where $\omega_0=(k_1/m)^{1/2}$ being a characteristic frequency taken as $\omega_0=13.04710^{12}\ s^{-1}$ and $\gamma=k_2/k_1=0.135$.

The diagonalisation of the dynamical matrix D(z, γ) for $z=\exp(iaq_x)$, leads to the propagating eigenmodes and the corresponding eigenvectors of the nanowire. The resulting dispersion curves may be given as a function of φ_x in the first BZ, where the dimensionless wave vector along the x direction is given as $\varphi_x=aq_x$, q_x is the reciprocal lattice wave-vector along the x direction in the first BZ.

It is well known that energy through the system can only propagate by means of traveling waves with a group velocity defined as $Vg=d\Omega/dq$, which is the speed of the energy transport. The phonon group velocity, one important parameter that can be found from the dispersion relation, is simply the slope of the branch on the dispersion curves for each frequency Ω.

4. Phonon transmission via a shaped joint nanostructure

Consider the scattering of the propagating modes in the Gold nanowire by the shaped joint nanostructure, as is depicted in Fig. 2a. In order to analyze the scattering it is necessary to identify the