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Monte Carlo simulations of phonon transport in Si nanowires with constrictions

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ABSTRACT

Heat conduction in silicon nanowires that exhibit a diameter constriction are studied from a Monte Carlo technique used to solve the phonon Boltzmann transport equation. Through the tailoring of the constriction shape, it is shown that thermal conductivity of the nanostructures can be lowered and adjusted. The phonon mean free path related to boundary scattering then becomes a key parameter. The calculation of the thermal conductance through the constriction is also performed and in the case of "steep" constriction, the ballistic and diffusive transport regimes through an aperture are recovered depending on the size of the constriction. Temperature dependence of the thermal conductivity in such constricted structures is addressed and dominant scattering processes are evaluated. Eventually, the case of a "long constriction" is simulated and a lowering of thermal conductivity, as compared to simple nanowires, is observed and discussed.

1. Introduction

During the past decade a broad attention has been paid to heat transport properties in nanostructured materials [1–4], and more specifically in semiconductors compounds that are used in several technologies. Structures such as nanofilms, nanowires or nanoporous media have been extensively studied, experimentally and numerically. In order to understand the physical mechanisms that underlie heat transfer in these specific structures, one needs to study heat carriers properties such as phonon dispersion relations, the phonon lifetime and the density of states (DOS). Using these basic inputs, thermal properties such as the thermal conductivity (TC) or the inter-facial thermal resistance (Kapitza resistance) can be appraised. In many applications tailoring TC through a dedicated processing is considered as the most convenient way to elaborate materials with high, low and/or anisotropic TC. For example, in polymers carbon nanotube (CNT) inclusions can help increase the TC [5]. Oppositely, in semiconductors, alloying, doping with substitution elements or nano-structuring are the best ways to reduce it [6,7]. In the latter case, several studies have pointed out that TC reduction can be addressed by increasing the phonon scattering. In this framework two regimes exist, the phonon wave confinement regime and the structure confinement. In the first case, the phonon wavelength is close to the characteristic length of the structure. For instance, in superlattices and phononic crystals, these wave effects lead to a modification of the dispersion properties (band folding) that reduces the material TC [8–10]. In the second case, the structure characteristic size is shortened but remains large when compared to the phonon wavelength. In that case, phonon boundary scattering is an important issue that rules heat transport. In the well known case of Si nanowires, TC can be decreased by at least an order of magnitude [11,12].

Recently, nanowires were engineered in order to enhance phonon confinement through the modulation of their diameter [13,14]. Models and simulations [15,16] were also developed to appraise the magnitude of the TC lowering assuming simple square cross-section modulated nanowires by means of kinetic theory or molecular dynamics. In these studies, cavities and constrictions are supposed to be the origin of the TC drastic decreases as the phonon group velocity is strongly lowered with the trapping of phonon modes. In this "abrupt" configuration (nanowire with rectangular modulation) heat flux, which is related to transported energy quanta along the nanowire axis, is strongly perturbed.

Furthermore, heat transport in constrictions is also a major issue which has been considered to described the thermal resistance between a nano-sized object and a surface in the case of

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non perfect contact [17–19]. This is typically the case in scanning thermal microscopy (SThM) where the edge of the tip is often modeled as a constriction between two dissimilar materials. Constrictions have also been investigated theoretically to understand the diffusive/ballistic transport mechanism occurring through small apertures [20–22]. In the latter studies, phonon diffraction in the case of very small apertures was modeled. Constrictions are also present in nanojunctions and are often parts of micro electromechanical systems (MEMS). Recently, it has been experimentally shown that controlling their shape and size is important to adjust heat transport properties for several applications [23].

Nanowires with realistic constrictions are difficult to simulate properly because of several numerical limitations. In molecular dynamics based studies, dealing with complex geometries and micrometer length scales cannot be simply done due to the currently available computational resources. On the other hand, modeling of phonon transport through the resolution of the Boltzmann transport equation (BTE) by finite volumes techniques is often limited to simple Cartesian or cylindrical geometries. In such an approach, the description of a realistic shape for a constriction might be challenging. Eventually, techniques based on the use of a transmission function to calculate heat flux through the constriction and the corresponding conductance, which are often faster, do not give information about temperature distribution in the nanostructures. Those issues or limitations are no longer existing when phonon motion and scattering is treated with the Monte Carlo (MC) simulation of the BTE. The present work is dedicated to the study of heat transfer through nanowires with different constriction shapes and lengths. Through MC numerical simulations, heat and temperature profiles in the nanostructures are recovered for different constriction profiles. Then, equivalent Fourier's conductance and TC are determined.

The paper is organized as follows. Following the introduction, theoretical models used to appraise the thermal conductance are recalled. Then, the constriction modeling is presented as well as the MC simulation tools used for numerical simulation of phonon transport. In Section 3, conductance and TC for different constriction shapes are discussed and compared to existing theory. The particular case of a long constriction, similar to a nanowire between two heat reservoirs is addressed in Section 3.4. Finally, conclusions and perspectives to this work are given.

2. Models and simulation tools

This section deals with models and simulations used to study constrictions in nanostructures. First, theoretical models giving expressions of the thermal conductance through apertures are recalled. Then, the model used in the framework of MC phonon transport is detailed.

2.1. Constriction models

Conductance or thermal resistance due to a "point contact" constriction can be theoretically assessed in two limiting cases, the diffusive limit and the ballistic limit. Those limits are characterized by the phonon scattering mean free path (mfp) Λ, compared to the characteristic size of the constriction. Usually for bulk materials, this mfp is appraised considering all the possible scattering mechanisms, namely the three phonon processes, Normal (N) and Umklapp (U), as well as the impurity or defect scattering. For bulk silicon, which is the material studied in the present work, at 300 K, Λ_b^{Si} is in the range of [170–250] nm according to the chosen phonon dispersion properties and the calculation method [24–26]. Yet, for nanowires the phonon mfp is mainly ruled by phonon confinement and boundary scattering. Thus, it is commonly accepted that $\Lambda_{nw} = d$, where d is the nanowire diameter.

2.1.1. Diffusive limit

In "the diffusive limit", the phonon mfp is smaller than the aperture of the constriction (minimum diameter) $\Lambda < d_{min}$. In this case, the Maxwell's formula [22] holds and the thermal conductance G_{dif} (or the thermal resistance R_{dif}) for a circular aperture reads

$$G_{dif} = \frac{1}{R_{dif}} = k d_{min} \tag{1}$$

where k is the thermal conductivity of the media on both sides of the constriction. Considering the Knudsen number Kn, defined as $Kn = \Lambda/d_{min}$, the diffusive limit corresponds to small values of Kn. When the shape of the constriction changes, the diffuse conductance also changes [20].

2.1.2. Ballistic limit

In "the ballistic limit", the phonon mfp is much larger than the constriction aperture $\Lambda > d_{min}$. In this case, the phonon transport across the constriction can be understood as the flow rate of gas molecules in the free molecular flow regime [20]. Two limit cases can be distinguished depending on the phonon dominant wavelength $\lambda_{dom}(T) \simeq h v_s/4.25 k_B T$ at a given temperature, where h is the Planck constant, v_s refers to the speed of sound (here 6500 m/s for Si), and k_B is the Boltzmann constant [13]. First, if the size of the aperture d_{min} is larger than λ_{dom} the conductance can be derived from the net heat flux through the constriction. Assuming constant group velocity and small temperature gradient on both sides of the constriction it reads

$$G_{bal} = \frac{1}{R_{bal}} = \frac{3kA}{4\Lambda} \tag{2}$$

where $A = \pi d_{min}^2/4$ is the cross section of the aperture. G_{bal} depends on the inverse of the phonon mfp. This expression was first derived from electron transport within constriction and named Sharvin conductance. In the second case (which will be not considered here), d_{min} is similar or smaller than λ_{dom} and diffraction shall be accounted for. In the present study, simulations are mostly carried out at 300 K, $\lambda_{dom}(T) \simeq 0.25$ nm and the smallest aperture diameter considered here is more than ten times larger: therefore, diffraction can be reasonably considered as negligible.

2.2. Monte Carlo simulation tool

Monte Carlo (MC) calculations of the phonon transport were performed using a dedicated home-built simulation tool. The basic specifications of the numerical method were extensively described in several papers [27,28] for bulk material and successfully derived for nanowires and nanoporous thin films [29,26,30]. The method lies on the resolution of the Boltzmann transport equation (BTE) in the frame of the relaxation time approximation (RTA). Bulk silicon dispersion properties have been used for the sampling of phonon frequency and group velocity, as well as for the calculation of the scattering relaxation times following the model proposed by Holland [31]. Relaxation time approximation is supposed to be valid as spatial discretization is chosen in order to ensure that sampled phonon do not cross several cells over a time step and thus have a non negligible probability to scatter. Besides, in the present work, most of the studied nanowire and constriction diameters are sufficiently large to ensure that bulk properties can be used for phonon transport. For the thinner nanowire (d = 28 nm), the dispersion properties within the constriction are probably different. For instance, when looking at molecular dynamic studies dealing