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Valentin Jean, S Fumeron, K Termentzidis, X Zianni, David Lacroix. Monte Carlo simulations of phonon transport in Si nanowires with constrictions. *International Journal of Heat and Mass Transfer*, Elsevier, 2015, 86, pp.648-655. <10.1016/j.ijheatmasstransfer.2015.03.041>. <hal-01578181>

HAL Id: hal-01578181

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Submitted on 29 Aug 2017

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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, 2, 3, 4], and more specifically in semiconductor 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)

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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, 9, 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 describe the thermal resistance between a nano-sized object and a surface in the case of non perfect contact [17, 18, 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, 21, 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 subsection 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, 25, 26]. Yet, for nanowires the phonon mfp is mainly ruled by phonon confinement and boundary scattering. Thus, it is commonly accepted that $\Lambda_{\text{nw}} = d$, where d is the nanowire diameter.

Diffusive limit

In “the diffusive limit”, the phonon mfp is smaller than the aperture of the constriction (minimum diameter) $\Lambda < d_{\text{min}}$. 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

$$G_{\text{dif}} = \frac{1}{R_{\text{dif}}} = kd_{\text{min}} \quad (1)$$

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

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 $\lambda_{\text{dom}}(T) \simeq hv_s/4.25k_B T$ 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

$$G_{\text{bal}} = \frac{1}{R_{\text{bal}}} = \frac{3kA}{4\Lambda} \quad (2)$$

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 300K, $\lambda_{\text{dom}}(T) \simeq 0.25$ 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 with this issue [32], for nanowires with diameters lower than 4 nm, supplementary modes at low frequencies with high wave-numbers appear. This means that phonon with lower energy and group velocity are dominant and thus heat transport should be lowered. Then in some peculiar cases of this study, the thermal conductivity and conductance might be a little bit overestimated.

The BTE for phonons is related to the variations of the distribution function $f(T, \mathbf{r}, p, \mathbf{K})$ which depends on time t , location \mathbf{r} , polarization p and wave vector \mathbf{K} . In the absence of external force, the BTE expression

according to the RTA assumption is a classical transport equation in which time variation of f plus the advection term equal a collisional term [33]

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{K}}\omega \cdot \nabla_{\mathbf{r}}f = \frac{f^0 - f}{\tau} \quad (3)$$

where $f^0(T, p, \mathbf{K}) = 1/[\exp(\hbar\omega(p, \mathbf{K})/k_B T) - 1]$ is the Bose-Einstein equilibrium distribution with \hbar the reduced Planck's constant. $\tau(\omega, p, T, \mathfrak{L})$ is the total phonon scattering relaxation time, which depends on the phonon dispersion properties, on the temperature and possibly on a characteristic length \mathfrak{L} . In the framework of MC modeling, Eq. (3) is solved in two steps. First, the advective part of the BTE is addressed (left hand side term) assuming that there is no scattering. A statistically representative population of phonons is drawn (frequency, polarization and group velocity) from a cumulative distribution function based on the phonon energy at a given temperature [28, 26]. Then each energy bundle is allowed to drift with respect to: i) its group velocity within the nanostructure, ii) the chosen time step Δt , iii) the internal reflections at boundaries. Secondly, the phonon scattering step is achieved considering the right hand side term of Eq. (3). The characteristic relaxation time is given according to the ‘‘Matthiessen’’ summation rule. It takes into account: normal (N), umklapp (U) and impurity (I) scattering rates according to M.G. Holland[31, 26] formalism. Knowing the energy distribution in the nanostructure one can compute in a control volume the energy and subsequently the temperature. Furthermore, phonon heat flux along the nanowire axis is given by

$$\varphi_z = \frac{1}{V} \sum_{i=1}^{i=N_b} \hbar\omega_i \times v_{gzi} \quad (4)$$

where V is the control volume, N_b the number of phonon energy bundles in V and v_{gzi} the group velocity in the z direction (nanowire axis) of the phonon with frequency ω_i . Then, considering the Fourier's formalism an equivalent thermal conductivity can be appraised $k = -\varphi_z \frac{\Delta z}{\Delta T}$. As all these points were already detailed in previous studies, technical issues concerning the sampling and the scattering procedure will not be recalled presently.

The major modification implemented in the MC simulation tool is about the handling of the geometry of constrictions. In the present work continuous function $R(z)$ are used to set the radius of the constricted nanowire as a function of the z coordinate, in the Cartesian coordinates it satisfies $x^2 + y^2 - R^2(z) = 0$. Using continuous functions makes easier the calculation of cross sections and control volumes, but also the boundary collision procedure. In the latter one, knowing the phonon location, its propagation direction and the shape of the domain one can easily extract from Newton-Raphson algorithm the intersection point where the phonon bundle crosses the external boundary of a constricted nanowire.

$$(x_{\text{ini}} + v_{gx}t_I)^2 + (y_{\text{ini}} + v_{gy}t_I)^2 - R^2(z_{\text{ini}} + v_{gz}t_I) = 0 \quad (5)$$

where t_I is the phonon travel time between its initial position $(x_{\text{ini}}, y_{\text{ini}}, z_{\text{ini}})$ and the intersection point (x_I, y_I, z_I) with the external boundary. From this point, the normal direction \mathbf{n}_I at the surface is computed

and the phonon is assumed to be diffusely reflected (sampling polar and azimuthal angles) in the hemisphere defined by \mathbf{n}_I .

$$\begin{aligned} n_{xI} &= -2x_I \\ n_{yI} &= -2y_I \\ n_{zI} &= 2R(z_I) \left. \frac{dR(z)}{dz} \right|_{z_I} \end{aligned} \quad (6)$$

2.3. Studied structures

Two geometries are presented in the paper, the “short” and the “long” constrictions, Figure (1). They are respectively defined by equations (7) and (8).

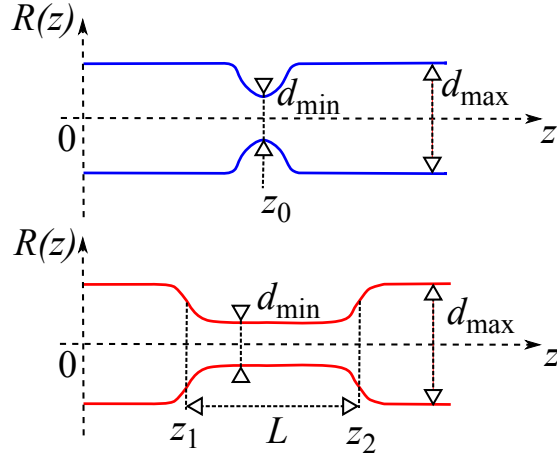


Figure 1: “Short” (blue) and “long” (red) constrictions; description of characteristic lengths and coordinates

$$R(z) = \frac{A}{1-B} \left[1 - \frac{B}{1+C(z-z_0)^2} \right] \quad (7)$$

$$\begin{aligned} R(z) &= A + B \{ \arctan[C^*(z-z_2)] \\ &\quad - \arctan[C^*(z-z_1)] \} \end{aligned} \quad (8)$$

A and B are constants that can be calculated using geometric conditions; $R(0) = d_{\max}/2$ and $R(z_0) = d_{\min}/2$ for Eq. (7), $R(0) = d_{\max}/2$ and $R(\frac{z_1+z_2}{2}) = d_{\min}/2$ for Eq. (8). L is the characteristic length of the “long constriction” (distance between z_1 and z_2). The parameters C and C^* related to the “steepness” of the constriction, for a large value of C or C^* the constriction is steep, while for a small value of C or C^* it is smooth. In the case of a short constriction the radius as a function of z becomes

$$R(z) = \frac{d_{\max}}{2} \left[1 - \frac{1-R_d}{1+C(z-z_0)^2} \right] \quad (9)$$

where $R_d = d_{\min}/d_{\max}$ stands for the diameter ratio.

3. Results and discussions

In this section phonon transport in short constrictions is addressed. Thermal conductivity of constricted nanowires and conductance of the constriction are studied as a function of: diameter ratio R_d , phonon mfp Λ , constriction steepness C and temperature T . We divided our results in three subsections.

3.1. Temperatures and heat fluxes

In this section, smooth and steep constrictions are studied and compared (Figure (2)). In order to compare TC simulation results to existing data, the chosen nanowire diameter is set to $d_{max}=115$ nm for which experimental results were reported by Li et al [11]. Here, $2 \mu\text{m}$ length nanowire are considered, and three cases are investigated: i) no constriction, ii) smooth constriction $C = 10^{14} \text{ m}^{-2}$, iii) steep constriction $C = 10^{16} \text{ m}^{-2}$ with $R_d = 0.5$. In Figure (3) are reported the heat flux density and the temperature profiles

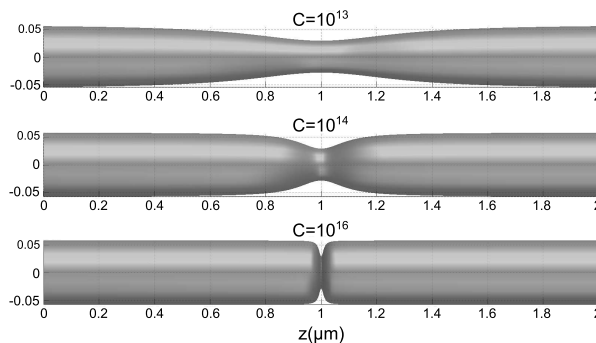


Figure 2: Different shapes of nanowire constriction; $L_z=2 \mu\text{m}$, $d_{max}=115$ nm, $d_{min}=57.5$ nm; top $C = 10^{13} \text{ m}^{-2}$, middle $C = 10^{14} \text{ m}^{-2}$ and bottom $C = 10^{16} \text{ m}^{-2}$

along the nanowire length. First, without any constriction, the TC is really close to the experimental measurement [11], the heat flux is maximum and the temperature profile almost linear as the phonon transport in the structure is diffusive (except in first and last cells where ballistic exchanges with boundaries, at fixed temperatures, can occur). For the constricted nanowires, temperature profiles exhibit drops in the vicinity of the constriction. The latter one seems to be more continuous in the case of a smooth constriction while it is abrupt for the steep one. As a consequence, heat flux density increases at the constriction location. The magnitude of the density heat flux peak shall be considered with caution as it depends on the spatial mesh choice. In the present calculations there are 40 control volumes with the same value of V to ensure reliable statistics in the MC procedure. It means that in the case of a steep constriction, no control volume is exactly inside the constriction, but rather on each side. On Figure (4) are plotted the heat flux density profiles for the smooth constriction with 40 and 180 cells. As discussed above, increasing the number of cells leads to an improved description of the peak maximum within the constriction. Nevertheless, the mean level remains the same, as well as the shape of the peak. Concerning the TC, there is a small increase between

both descriptions as the maximum heat flux is larger for 180 cells. Concerning the mean TC of constricted

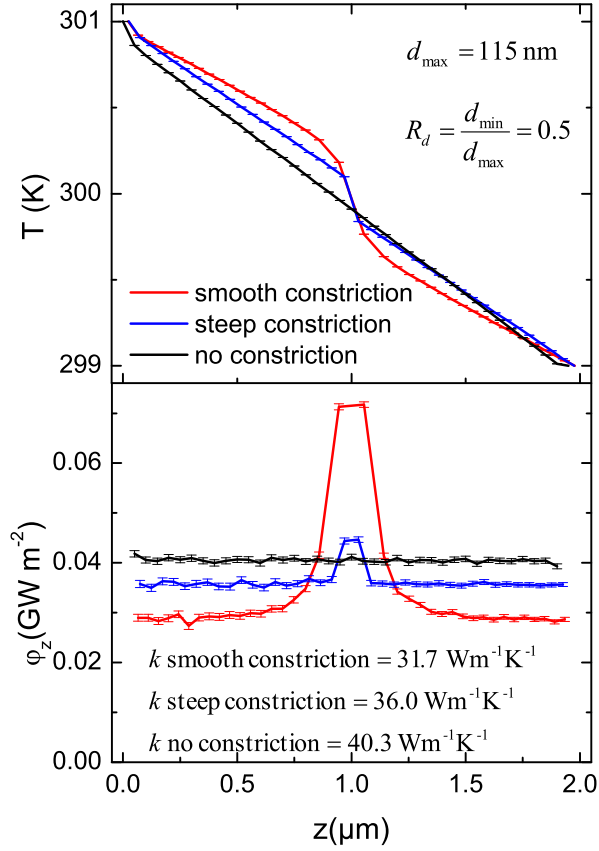


Figure 3: Heat flux density and temperature profiles, $d_{\text{max}}=115 \text{ nm}$, $R_d = 0.5$; no constriction (black), smooth constriction $C = 10^{14} \text{ m}^{-2}$ (red), steep constriction $C = 10^{16} \text{ m}^{-2}$ (blue)

nanowires, it obviously decreases. This decrease is more important for the smooth one. This behavior can be explained from the phonon boundary scattering mfp calculation. When the constriction is smooth, phonon mfp for boundary scattering is getting smaller and thus the thermal conductivity. This point is addressed in the following.

3.2. Thermal conductivity

3.2.1. Steepness dependence

First, the dependence of the TC with respect to the phonon mfp in constricted nanowire is addressed through the steepness of the constriction. The latter parameter can be obtained numerically and analytically. Using the MC simulation tool, a ray tracing (RT) experiment was carried out. For such a case, a very large amount of phonons is sampled in the whole structure and collisions with the nanowire surface envelope are counted during one small time step. The ratio of the number of collision N_{coll} to the total number of drawn phonon N_{tot} is equal to the collision probability. Thus, using the same technique as in Lacroix et al [29],

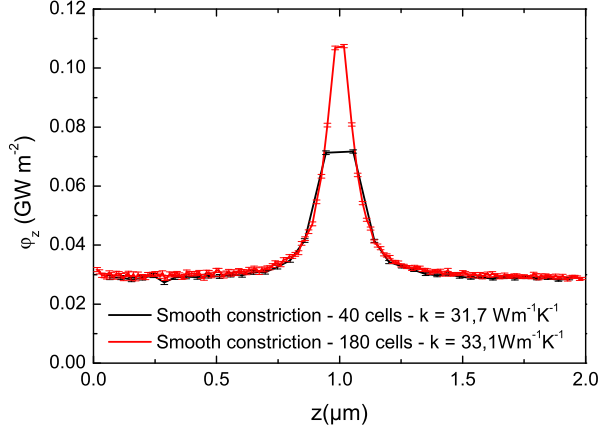


Figure 4: Heat flux density as a function of the number of control volumes, $d_{\max}=115$ nm, $R_d = 0.5$, $C = 10^{14}$ m $^{-2}$; 40 cells (black), 180 cells (red)

one can appraise Λ_{RT} from numerical data as

$$\Lambda_{RT}(\omega, p, d, C) = \frac{v_g \Delta t}{\ln \left[\frac{N_{\text{tot}}(\omega, p)}{N_{\text{tot}}(\omega, p) - N_{\text{coll}}(\omega, p)} \right]} \quad (10)$$

where ω stands for the frequency and p the polarization. Simulation results show that there is no frequency or polarization dependence, but the mfp naturally varies according to the shape of the nanowire. Another way to express a particle mfp subject to diffuse transport was proposed by Blanco and Fournier [34]. This analytical expression solely depends on the volume of the structure V_{tot} and the surface S_{env} of the contour envelope and it reads

$$\Lambda_{\text{th}}(\omega, p, d, C) = \frac{4V_{\text{tot}}}{S_{\text{env}}} \quad (11)$$

Both expressions were used to calculate Λ for the previously studied nanowires using different values of the steepness parameter C . Results are reported in Table (1). The calculated mfp by both methods are in quite

Table 1: Variation of the phonon mfp for boundary scattering as the function of the steepness parameter C using Eq. (10) and Eq. (11); $d_{\max}=115$ nm, $R_d = 0.5$; Λ is given in nm.

C	10^{13}	10^{14}	$5 \cdot 10^{14}$	10^{15}	$5 \cdot 10^{15}$	10^{16}	$5 \cdot 10^{16}$	10^{17}
Λ_{RT}	96.6	106.4	108.3	110.1	110.6	110.9	110.9	111.0
$\Lambda_{\text{th}}[34]$	95.2	104.5	109.3	110.8	113.1	113.7	114.5	114.7

good agreement. In the case of the analytic solution, for large values of C , the constriction is a very localized modification of the geometry (aperture of diameter d_{\min} in the cylinder of diameter d_{\max}) and thus the mfp tends to d_{\max} . For smooth constrictions (i.e. small values of C), the mfp becomes smaller as the geometry looks like a ‘‘conical’’ constriction. On figure (5), thermal conductivity results are reported as a function of Λ . Using this description obviously shows that TC is linearly varying with the mfp. Furthermore, for the

largest value of C , where the constriction is similar to a single aperture in the nanowire, and for $R_d=0.5$, the TC is reduced by 10% as compared to the cylindrical nanowire.

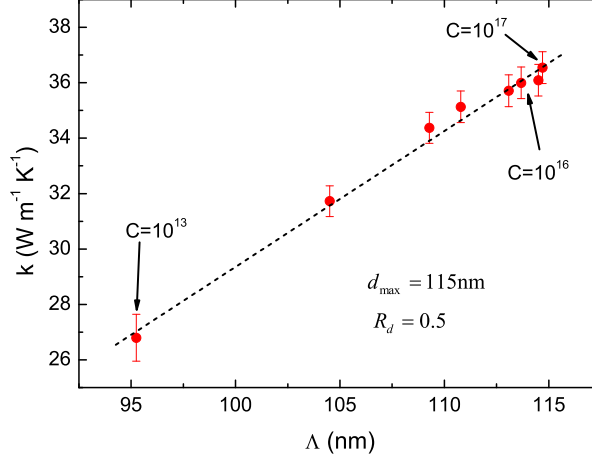


Figure 5: Thermal conductivity as a function of the mfp, $d_{\max}=115$ nm, $R_d = 0.5$

3.2.2. Diameter ratio dependence

On the basis of the previously adopted methodology, the TC is calculated for several nanowire diameters and constriction ratios R_d . In Figure (6) are reported the MC simulation results for six values of d_{\max} and three constriction ratio. Calculations are compared to the TC of a nanowire without constriction. First, the

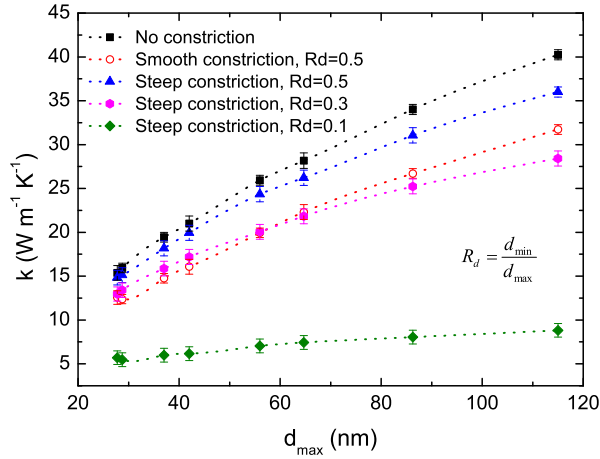


Figure 6: Thermal conductivity as a function of the nanowire diameter and the constriction ratio; $d_{\max}=[37; 42; 56; 65; 86; 115]$ nm, $R_d=[0.1; 0.3; 0.5; 1.0]$

TC of non constricted nanowire (black squares) is always larger than the ones of nanowires with constriction. Moreover, it can be observed that the steepness of the constriction affects the calculated TC whatever the

nanowire diameter is. This is due to the reduction of the phonon mfp for smooth constrictions discussed previously. The second point is that the constriction ratio R_d lowering also induces the lowering of TC. This effect is more important for nanowires with large diameters for which phonon mfp is more affected by the constriction. Besides, it can be noted that there is a strong decrease of the TC when R_d is small (here we have $R_d=0.1$). In the latter case, the TC remains almost constant for all the studied diameters. For such small values of R_d , transport is ballistic through the aperture. Here, the phonons transmitted through the constriction are propagating along z axis. This point will be studied in more details in the next subsection dealing with the conductance. It shall be noted that simulations done for small d_{\max} and R_d values, are in the limit of the BTE resolution with our technique since dispersion properties in the vicinity of the constriction are likely to be modified. Besides, several system lengths were simulated (here $L_z=2 \mu\text{m}$) and no difference was found in the calculated TC. Here, the characteristic mfp is of the order of the nanowire diameter, that is much lower than its length, and thus thermal transport is diffusive.

3.2.3. Temperature dependence

Finally, the temperature dependence of TC in constricted nanowires is discussed. In Figure (7) is plotted the TC versus temperature for a nanowire with $d_{\max}=115 \text{ nm}$, $C = 10^{16} \text{ m}^{-2}$ and two constriction ratios (0.5 and 0.3) over the temperature range $30 < T < 600 \text{ K}$. The temperature dependence for all the studied

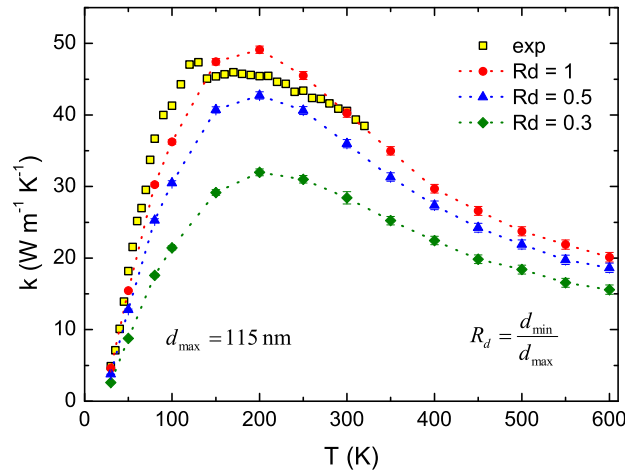


Figure 7: Thermal conductivity as a function of the temperature; $d_{\max}=115 \text{ nm}$, $C = 10^{16} \text{ m}^{-2}$, $R_d=[0.3;0.5; 1.0]$; yellow squares stand for experimental data taken from Li et al[11]

geometries (with and without constriction) follows the same trends as in bulk Si, with a noticeable decrease of the TC due to boundary scattering. In the case of the nanowire with no constriction, simulation data are in quite good agreement with the one of Li et al[11]. Once again, TC of constricted nanowire is always lower than the one of regular nanowire. Nevertheless, the decrease is more important for temperatures between 50 K and 400 K. Above this temperature the phonon scattering due to phonon-phonon interactions is no

more negligible as compared to the one of boundary scattering and a competition between both mechanisms occurs. Such dependence to the temperature paves the way to possible thermal rectification by adjusting the shape of the constriction and the temperature of thermal baths on both sides of the nanowire. For temperatures below 30 K, MC calculations are not carried out since phonon wavelength becomes larger and closer to the constriction aperture leading to potential diffraction effects.

3.3. Constriction conductance

In order to address more precisely the impact of the constriction itself on the phonon transport, the thermal conductance $G = \frac{\Phi}{\Delta T}$ is calculated using a simple model of thermal resistance in series. We suppose that the total thermal resistance of the constricted nanowire is the sum of two resistances $R_{\text{tot}} = R_{\text{nw}} + R_C$, one for the regular nanowire plus one corresponding to the constriction (they are respectively the analogs of frictional and singular head losses in fluid mechanics). In terms of conductance it reads

$$G_C = \frac{G_{\text{tot}} \times G_{\text{nw}}}{G_{\text{nw}} - G_{\text{tot}}} \quad (12)$$

Using the Eq. (12) does not require to define the temperature gradient and the heat flux in the constrictions; the exact location of the constriction boundaries being subject to different interpretation in the case of smooth and steep profiles, as it is shown in Figure (3).

In Figure (8) are reported the thermal conductance of the constriction for different values of the nanowire diameter and of the diameter ratio. Several points can be observed. First concerning the steepness of the constriction, it can be noted that in the case of the smooth one, there is no visible agreement with the theory for diffusive and ballistic limits. This is logical since Maxwell (diffusive) and Sharvin (ballistic) models are related to a point contact constriction (single aperture between two structures). This is not the case for the nanowire with $C = 10^{14} \text{ m}^{-2}$ where the shape of constriction is hyperboloid like. In the case of a steep constriction, MC calculations of the conductance vary between both limits as the simulated geometry is similar to the one of the point contact model. Secondly, for a small diameter ratio ($R_d=0.1$), the conductance trend is obviously close to the one in the ballistic limit. It is in agreement with remarks made in the previous section about the TC (Figure (6)). As the diameter of the nanowire gets larger, as well as the constriction ratio, the constriction conductance reaches the diffusive limit.

3.4. Long constrictions

We now discuss the case of a long constriction, defined as a nanowire with diameter d_{min} connected by constriction to larger nanowires with diameter d_{max} (see Figure (1)). The length L of the constriction is one of the studied parameters. The other one is the diameter ratio R_d .

In figure (9) are plotted the results for long constrictions and comparisons with regular cylindrical nanowires as well as nanowires with short constrictions. The maximum diameter is constant $d_{\text{max}}=115 \text{ nm}$, the diameter ratio are $R_d=[0.25; 0.50; 0.75; 1.00]$ and the length $L=[500 ;1000; 1500; 2000] \text{ nm}$. On both

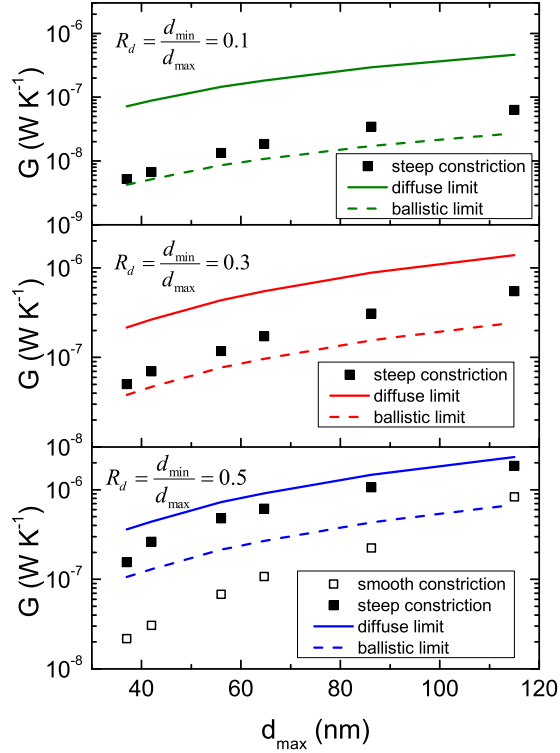


Figure 8: Constriction thermal conductance as a function of the nanowire diameter and the constriction ratio; $d_{\max}=[37; 42; 56; 65; 86; 115]$ nm, $R_d=[0.1; 0.3; 0.5]$; black squares $C = 10^{16} \text{ m}^{-2}$, open squares $C = 10^{14} \text{ m}^{-2}$; comparisons to the ballistic limit Eq. (2) and diffusive the limit Eq. (1)

sides of the constriction the length of d_{\max} nanowires is equal to 500 nm. The first observation concerns the length of the constriction. When L is larger than 500 nm, there is almost no change in the calculated mean TC of the nanostructure, whatever the diameter ratio R_d is. The second important point is that TC of long constriction systems is always smaller than those corresponding to short constrictions with the same other geometrical characteristics (green diamonds in figure (9)). It can be recalled that in the present work, phonon transport is diffusive and consequently, difference in TC is due to the new internal thermal resistance. This is confirmed by the comparison of TC values of long constrictions with the pristine nanowire ones. For each R_d value, ($R_d = 0.75 \rightarrow d_{\min} = 86.25$ nm; $R_d = 0.5 \rightarrow d_{\min} = 57.5$ nm; $R_d = 0.25 \rightarrow d_{\min} = 28.75$ nm), the TC of long constrictions is also lower than these of the nanowires with diameter d_{\min} (yellow hexagons). Nevertheless, for long constriction structures, if TC is calculated at the central part of the nanowire, where $d = d_{\min}$, the pristine nanowire TC is recovered confirming the occurrence of thermal resistance. Another interesting issue is that the TC of a thin nanowire between two larger ones (case where $R_d=0.25$) leads to

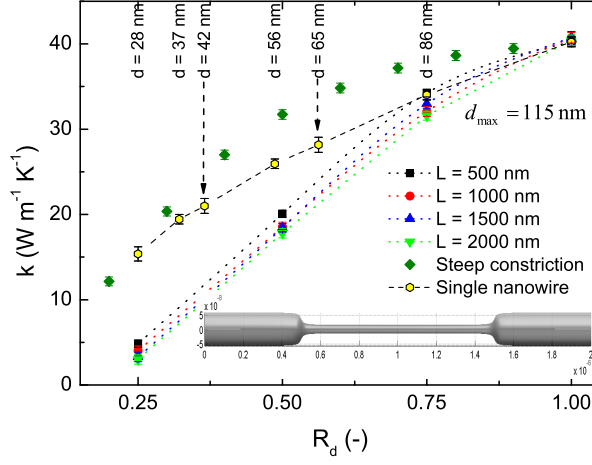


Figure 9: Long constriction thermal conductivity as a function of the constriction ratio and the length of the constriction; $d_{max}=115$ nm, $R_d=[0.25; 0.50; 0.75; 1.00]$, $L=[500; 1000; 1500; 2000]$ nm; green diamonds steep constriction $C^* = 10^8$ m⁻¹; yellow hexagons pristine nanowires

values three times lower when compared to the regular nanowire of diameter $d_{min} = 28.75$ nm. This lowering is similar to what was observed by Li et al[11] and attributed to nanowire roughness [12]. Therefore, the presence of heat reservoirs on both sides of the inner nanowire with the small diameter seems to affect the overall thermal conductivity and should be accounted for in thermal properties measurements at nanoscales. Such behaviour is also confirmed by calculations achieved on modulated nanowires [16, 30], where TC of a structure that alternates large and small diameters is lower than the one of the corresponding small diameter.

4. Conclusions

Monte Carlo simulations of phonon transport in nanowires with a constriction were performed and discussed. Thermal conductivity as well as thermal conductance have been appraised and compared to available experimental data and literature models. A detailed study of the constriction geometry was carried out. Steepness of the constriction and the magnitude of diameter reduction were first addressed. It has been shown that the TC behavior is ruled by the phonon mean free path related to boundary scattering. The latter one can be evaluated analytically. Concerning the magnitude of the constriction, two regimes exist. When the diameter of constriction is large, there is little resistance to phonon transport and the regime is “diffusive”. Oppositely, when the diameter of constriction is small, thermal conductivity remains quite uniform and the transport is “ballistic”. This behavior is also observed for the thermal conductance that varies between these two limit regimes when the constriction is steep. In the latter case, the constriction fit to the “point contact” model and the associated conductance can be simply appraised from the thermal conductivity of the nanowire. In such a case conductance is a linear function of the Knudsen number and of the thermal conductivity of the bounding material as suggested in former studies

like [18]. Otherwise, we show that in the case of smooth constriction, the conductance is no longer described by the Maxwell or Sharvin models. The temperature dependence was also investigated, as expected, the impact of the constriction on the TC is more or less pronounced as the the phonon mfp is dominated by boundary scattering or three phonons processes. TC being significantly reduced by constriction occurrence at low temperatures that at high. The last part of this work is about “long constrictions” that can be related to a nanowire between two heat reservoirs. For such structure, the TC is lower than in the case of a single nanowire. It puts forward the importance of thermal resistances induced by the constrictions. This behavior confirms previous studies on modulated nanowire and gives useful insights to understand thermal properties measurements experimentally achieved.

This work will be continued considering modulations and asymmetric constrictions that could exhibit thermal rectification. Moreover, phonon transport within constrictions, and especially frequency and wavelength dependence will be deeper investigated.

5. Acknowledgements

People involved in this work acknowledge invited professorship of the University of Lorraine (LEMTA) for Pr X. Zianni and the project “SiMoNE”, PEPS Mirabelle 2013 funded by CNRS and the University of Lorraine.

- [1] D. G. Cahill, W. K. Ford, K. E. Goodson, G. D. Mahan, A. Majumdar, H. J. Maris, R. Merlin, and S. R. Phillpot. Nanoscale thermal transport. *Journal of Applied Physics*, 93(2):793, 2003.
- [2] D. G. Cahill, P. V. Braun, G. Chen, D. R. Clarke, S. Fan, K. E. Goodson, P. Keblinski, W. P. King, G. D. Mahan, and A. Majumdar. Nanoscale thermal transport. II. 2003–2012. *Applied Physics Reviews*, 1(1):011305, 2014.
- [3] T. Luo and G. Chen. Nanoscale heat transfer – from computation to experiment. *Physical Chemistry Chemical Physics*, 15(10):3389, 2013.
- [4] N. Yang, X. Xu, G. Zhang, and B. Li. Thermal transport in nanostructures. *AIP Advances*, 2(4):041410, 2012.
- [5] Zhidong Han and Alberto Fina. Thermal conductivity of carbon nanotubes and their polymer nanocomposites: A review. *Progress in Polymer Science*, 36(7):914–944, July 2011.
- [6] M. Maldovan. Thermal energy transport model for macro-to-nanograin polycrystalline semiconductors. *Journal of Applied Physics*, 110(11):114310, 2011.
- [7] Z. Wang, J. E. Alaniz, W. Jang, J. E. Garay, and C. Dames. Thermal Conductivity of Nanocrystalline Silicon: Importance of Grain Size and Frequency-Dependent Mean Free Paths. *Nano Letters*, 11(6):2206–2213, June 2011.
- [8] S. Ren and J. Dow. Thermal conductivity of superlattices. *Physical Review B*, 25(6):3750–3755, March 1982.
- [9] B. Yang and G. Chen. Partially coherent phonon heat conduction in superlattices. *Physical Review B*, 67(19), May 2003.
- [10] N. Zen, T. A. Puurtinen, T. J. Isotalo, S. Chaudhuri, and I. J. Maasilta. Engineering thermal conductance using a two-dimensional phononic crystal. *Nature Communications*, 5, March 2014.
- [11] D. Li, Y. Wu, P. Kim, L. Shi, P. Yang, and A. Majumdar. Thermal conductivity of individual silicon nanowires. *Applied Physics Letters*, 83(14):2934, 2003.
- [12] R. Chen, A. I. Hochbaum, P. Murphy, J. Moore, P. Yang, and A. Majumdar. Thermal Conductance of Thin Silicon Nanowires. *Physical Review Letters*, 101(10), September 2008.
- [13] C. Blanc, A. Rajabpour, S. Volz, T. Fournier, and O. Bourgeois. Phonon heat conduction in corrugated silicon nanowires below the Casimir limit. *Applied Physics Letters*, 103(4):043109, 2013.
- [14] J. Maire and M. Nomura. Reduced thermal conductivities of Si one-dimensional periodic structure and nanowire. *Japanese Journal of Applied Physics*, 53(6S):06JE09, June 2014.
- [15] Denis L. Nika, Alexandr I. Cocemasov, Dmitrii V. Crismari, and Alexander A. Balandin. Thermal conductivity inhibition in phonon engineered core-shell cross-section modulated Si/Ge nanowires. *Applied Physics Letters*, 102(21):213109, 2013.
- [16] K. Termentzidis, T. Barreateau, Y. Ni, S. Merabia, X. Zianni, Y. Chalopin, P. Chantrenne, and S. Volz. Modulated SiC nanowires: Molecular dynamics study of their thermal properties. *Physical Review B*, 87(12), March 2013.
- [17] L. Shi and A. Majumdar. Thermal Transport Mechanisms at Nanoscale Point Contacts. *Journal of Heat Transfer*, 124(2):329, 2002.
- [18] S. Volz and P.-O. Chapuis. Increase of thermal resistance between a nanostructure and a surface due to phonon multireflections. *Journal of Applied Physics*, 103(3):034306, 2008.

- [19] D. Singh, J. Y. Murthy, and Timothy S. Fisher. Phonon Transport Across Mesoscopic Constrictions. *Journal of Heat Transfer*, 133(4):042402, 2011.
- [20] R. Prasher. Predicting the Thermal Resistance of Nanosized Constrictions. *Nano Letters*, 5(11):2155–2159, November 2005.
- [21] R. Prasher, T. Tong, and A. Majumdar. Diffraction-limited phonon thermal conductance of nanoconstrictions. *Applied Physics Letters*, 91(14):143119, 2007.
- [22] Sanjoy K. Saha and Li Shi. Molecular dynamics simulation of thermal transport at a nanometer scale constriction in silicon. *Journal of Applied Physics*, 101(7):074304, 2007.
- [23] L. Jalabert, T. Sato, T. Ishida, H. Fujita, Y. Chalopin, and S. Volz. Ballistic Thermal Conductance of a Lab-in-a-TEM Made Si Nanojunction. *Nano Letters*, 12(10):5213–5217, October 2012.
- [24] G. Chen. Thermal conductivity and ballistic-phonon transport in the cross-plane direction of superlattices. *Physical Review B*, 57(23):14958, 1998.
- [25] A. Minnich and G. Chen. Modified effective medium formulation for the thermal conductivity of nanocomposites. *Applied Physics Letters*, 91(7):073105, 2007.
- [26] V. Jean, S. Fumeron, K. Termentzidis, S. Tutashkonko, and D. Lacroix. Monte Carlo simulations of phonon transport in nanoporous silicon and germanium. *Journal of Applied Physics*, 115(2):024304, January 2014.
- [27] S. Mazumder and A. Majumdar. Monte Carlo Study of Phonon Transport in Solid Thin Films Including Dispersion and Polarization. *Journal of Heat Transfer*, 123(4):749, 2001.
- [28] J.-P. M. Péraud and N. G. Hadjiconstantinou. Efficient simulation of multidimensional phonon transport using energy-based variance-reduced Monte Carlo formulations. *Physical Review B*, 84(20):205331, November 2011.
- [29] D. Lacroix, K. Joulain, D. Terris, and D. Lemonnier. Monte Carlo simulation of phonon confinement in silicon nanostructures: Application to the determination of the thermal conductivity of silicon nanowires. *Applied Physics Letters*, 89(10):103104, 2006.
- [30] Xanthippi Zianni, Valentin Jean, Konstantinos Termentzidis, and David Lacroix. Scaling behavior of the thermal conductivity of width-modulated nanowires and nanofilms for heat transfer control at the nanoscale. *Nanotechnology*, 25(46):465402, November 2014.
- [31] M. G. Holland. Analysis of lattice thermal conductivity. *Physical Review*, 132(6):2461, 1963.
- [32] M.-J. Huang, C.-C. Weng, and T.-M. Chang. An investigation of the phonon properties of silicon nanowires. *International Journal of Thermal Sciences*, 49(7):1095–1102, July 2010.
- [33] Neil W. Ashcroft and David N. Mermin. *Solid state Physics*. Saunders College, Philadelphia, 1976.
- [34] S. Blanco and R. Fournier. An invariance property of diffusive random walks. *EPL (Europhysics Letters)*, 61(2):168, 2003.