Effect of Constriction on Phonon Transport in Silicon Thin Films and Nanowires

Jay Dulhani and Bong Jae Lee

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea

ABSTRACT

Technological advancement has made manufacturing of various nanostructures possible. Thermal transport in such nanostructures is fundamentally different from macroscale. Initial studies have indicated that thermal properties of these nanostructures also depend on its geometry. Hence, it is possible to tailor nanostructure geometry to achieve targeted thermal properties. In the present work, thermal transport in (a) constricted thin films and (b) constricted nanowires is studied using gray phonon Boltzmann transport equation (BTE) for a widerange of constriction ratio. Finite volume method is used to numerically solve the BTE with the relaxation time approximation. We show in this paper that by varying the degree of constriction, thermal conductivity of thin films and nanowires can be altered significantly. Thin films and nanowires are found to respond differently to constriction.

1. Introduction

Phonons are quantized lattice vibrations that are the dominant heat carrier in semiconductor and dielectric materials. Phonons’ cumulative response governs nanostructures thermal property. Thermal transport in nanostructures have been a subject of interest in both theoretical and practical applications.[1,2] Understanding and regulating phonon transport have thus become a major challenge for efficient thermal management of these nanostructures. Different applications need nanostructures with different set of thermal properties. For example, thermoelectronic devices require material with low-thermal conductivity,[3,4] whereas vice versa is true for LEDs.[5,6] In this regard, researchers are trying to control thermal conductivity of nanostructure as per the need. Initial studies have indicated that this can be achieved through various ways, for example, by doping,[7] by varying surface roughness,[8–10] or by engineering nanostructure geometry,[11–15] etc.

By engineering nanostructure geometry, it is also possible to alter the interaction between phonon and nanostructure boundary (i.e. phonon boundary scattering), which governs the thermal transport in nanostructure. Li et al. [11] demonstrated strong diameter dependence of thermal conductivity of silicon nanowire due to the phonon-boundary scattering. Similar observation was reported by Maire and Nomura [12] and Bera [13]. Heron et al. [14] also studied geometry-induced effect on phonon transport in nanowires. They observed significant reduction in thermal conductance by introducing a serpentine structure in a straight nanowire. Recently, Jean et al. [15] studied thermal transport in nanowires with diametric constriction at the center. They observed that by tailoring the constriction shape, thermal conductivity of nanowires can be adjusted.

It is obvious from the preceding discussion that by engineering nanostructure geometry, thermal transport in nanostructure can be altered. On the other hand, there...
are very few publications available in the literature which emphasize on the effect of constriction on thermal transport in nanostructure. To the author’s best knowledge, study focusing on the effect of constriction on tapered thin films and tapered nanowires has not been carried out yet. These configuration not only find strong resemblance with thermal scanning probe tip (see Figure 1) but also have significant application in microelectronics, thermoelectronics, and other emerging areas. Hence, there is a strong need for an investigation.

The present study aims to understand geometry induced effect on phonon transport in tapered nanostructures by solving Boltzmann transport equation (BTE). Gray phonon BTE is used for the present study. Over the years, gray phonon BTE has been used to study a variety of problems in sub-micron domain, for example, phonon transport across mesoscopic constrictions,[16] gas–phonon coupling,[17] and in calculation of thermal boundary resistance.[18] Thus, gray BTE is a reliable choice for the present objective.

2. Overview of numerical method

2.1. Formulation

The schematic of geometrical configuration for present study is shown in Figure 2. Thin film (i.e. two-dimensional) or nanowire (i.e. axisymmetric) is placed between two thermal reservoirs; thus, maintaining a constant temperature difference between its end. Length of the nanostructure is \( L \). The width (or diameter) of broad end of tip is \( W_{\text{max}} \) (or \( d_{\text{max}} \)), whereas, width (or diameter) of narrow end of tip is \( W_{\text{min}} \) (or \( d_{\text{min}} \)) for thin film (or for nanowire). Broad end is maintained at temperature \( T_1 \), while the other end is at temperature \( T_2 \).

BTE governs phonon transport in nanostructures. At steady state, BTE can be written as [19]

\[
\nabla \cdot (\hat{s} v_g e'') = \left( \frac{\partial e''}{\partial t} \right)_{\text{scat}} \tag{1}
\]

where \( e'' \) is the net phonon energy density at position \( \vec{r} \) in the direction \( \hat{s} \), \( v_g \) is the phonon group velocity, and \( \left( \frac{\partial e''}{\partial t} \right)_{\text{scat}} \) represents the change in the phonon energy density due to inelastic scattering. The scattering term has complex dependence on various parameters; thus, resolving it is complicated and computationally expensive. In order to overcome this challenge, several approximation techniques have been developed. In this work, the relaxation time approximation is used to resolve scattering term. The steady-state gray BTE with the relaxation time approximation is expressed as

\[
\nabla \cdot (\hat{s} v_g e'') = \frac{e^0 - e''}{\tau} \tag{2}
\]

where \( \tau \) is phonon relaxation time and \( e^0 \) is the equilibrium energy density. The phonon energy density at equilibrium is determined from the following equation:

\[
4\pi e^0 = \int_{4\pi} e'' \, d\Omega \tag{3}
\]

where the integration is conducted over the solid angle \( \Omega \). With the assumption that volumetric heat capacity is constant due to small temperature difference in the domain, temperature field can be obtained from equilibrium phonon energy density from the following equation:

\[
e^0(\vec{r}) = C \frac{T(\vec{r})}{4\pi} \tag{4}
\]

where \( C \) is specific heat and \( T(\vec{r}) \) is lattice temperature corresponding to position vector \( \vec{r} \).

2.2. Boundary conditions

In the present study, three boundary conditions (i.e. thermalizing, diffuse, and specular) are considered as briefly explained in the following. Under thermalizing boundary condition, the energy density of phonons entering the domain from thermalizing boundary at temperature \( T_b \) is given by \( e'' = e^0 = C \frac{T_b}{4\pi} \). Regarding diffuse boundary condition, the energy density of phonons entering the domain (i.e. \( \hat{s} \cdot \hat{n} < 0 \), where \( \hat{n} \) is the surface normal
Figure 2. Schematic of geometrical configurations: (a) tapered thin film and (b) tapered nanowire.

vector) is given by:

\[ e''(\hat{s}) = \frac{1}{\pi} \int_{\hat{s} \cdot \hat{n} > 0} e''(\hat{s} \cdot \hat{n}) \, d\Omega \quad (5) \]

On the other hand, under specular boundary condition, for directions incoming to the domain, following condition is applied:

\[ e''(\hat{s}) = e''(\hat{s}_r) \quad (6) \]

where \( \hat{s}_r = \hat{s} - 2(\hat{s} \cdot \hat{n})\hat{n} \). For directions outgoing to the domain (i.e. \( \hat{s} \cdot \hat{n} > 0 \)), \( \nabla \cdot (\vec{e''}) = 0 \) is applied to all the boundary conditions.

2.3. Method of solution

Over the years, several numerical methods have been developed to solve BTE, such as finite volume method (FVM),\[20\] discrete ordinate method,\[21\] lattice Boltzmann method,\[22,23\] and Monte Carlo method,\[24\] etc. In the present work, we will be using FVM to solve gray phonon BTE. The advantages of FVM include good solution accuracy, consistency, reasonably small computational time, and ability to handle complex geometry.\[25\]

Cartesian model is used to simulate thermal transport in thin film [refer to Figure 2(a)], whereas axisymmetric model is applied for nanowire [refer to Figure 2(b)]. Detailed solution procedures for cartesian \[20\] and axisymmetric \[26,27\] coordinate system are already available in literature. Hence, they are not repeated here. As phonons inherently travel in three dimensions, discretization is performed in both the spatial and angular domains.\[20\]

The spatial domain is discretized into non-overlapping control volumes and the angular domain at any location is discretized into non-overlapping control angles (refer to Figure 3). The BTE in any given direction is integrated over the control volume and the control angle yielding linear set of algebraic equations in energy density. These are solved using the tridiagonal matrix algorithm. Once
the Knudsen number is defined as $Kn = \frac{\Lambda}{\lambda}$, where $\Lambda$ is the mean free path of phonons, and $L$ is a characteristic length. The length of the domain ($L$) is changed to vary Knudsen number, while the width of film ($W$) is maintained at $1$ m/s, mean free path $\Lambda = 260.4$ nm, and specific heat $C = 0.93 \times 10^6$ J/m$^3$·K.

3. Results and discussion

Thermophysical properties of silicon required for BTE simulations are calculated following Chen’s phonon branch averaging procedure.[28] The thermophysical properties used are (at 300 K): group velocity $v_g = 1804$ m/s, mean free path $\Lambda = 260.4$ nm, and specific heat $C = 0.93 \times 10^6$ J/m$^3$·K.

3.1. Code validation

For the purpose of validation, simulations are performed for steady-state heat conduction in a silicon thin film. The Knudsen number is defined as $Kn = \frac{\Lambda}{\lambda}$, where $\Lambda$ is the mean free path of phonons, and $L$ is a characteristic length. The length of the domain ($L$) is changed to vary Knudsen number, while the width of film ($W$) is maintained at $1$ m/s, mean free path $\Lambda = 260.4$ nm, and specific heat $C = 0.93 \times 10^6$ J/m$^3$·K.

3.2. Effect of constriction

For all results presented here by, nanostructure’s wall is assumed to be diffusely reflecting. As far as discretization is concerned, angular domain of $2\pi$ (i.e. $0 \leq \theta \leq \pi$, $0 \leq \phi \leq \pi$; due to symmetry) is discretized into $128 \times 128$ non-overlapping control angles. As far as spatial domain is concerned, all computations are performed with 3000 control volumes. Further refinement in spatial and angular discretization does not bring any reasonable change to the computation accuracy.

3.2.1. Variation in thermal conductivity

The effect of constriction on phonon transport begins by first considering, phonon transport in constricted thin film (refer to Figure 2). The length of film, $L = 1500$ nm. The width of the broad end of the film, $W_{\text{max}} = 200$ nm, and the width of the narrow end, $W_{\text{min}}$, is varied from 40 to 200 nm. The length scales chosen are consistent with the previous studies.[15,30] On the other hand the transport in the in-plane direction is near ballistic. Figure 5 represents variation in thermal conductivity of silicon thin film with constriction ratio ($C_r = W_{\text{min}}/W_{\text{max}}$). Using kinetic theory, thermal conductivity of bulk–silicon (at 300 K) can be recovered, and is equal to $145.62$ W/m·K. It can be observed that unconstricted thin film (i.e. $C_r = 1$) has thermal conductivity much smaller than the bulk. This can be attributed to significant phonon-boundary scattering in thin film which otherwise is absent in bulk. Reduction in thermal conductivity with reduction in constriction ratio is also observed. Reduction in constriction ratio leads to increase in area to volume ratio of thin film. Higher area to volume ratio implies higher phonon boundary scattering. This enhancement in phonon-boundary scattering is responsible for suppression of lattice thermal conductivity.[31] Secondly, the effect of constriction on thermal transport in silicon nanowire is studied. By keeping $L = 1500$ nm and $d_{\text{max}} = 200$ nm, diameter of narrow end ($d_{\text{min}}$) is varied from 40 to 200 nm. The variation in thermal conductivity of constricted nanowire with constriction ratio ($C_r = d_{\text{min}}/d_{\text{max}}$) is shown in Figure 5. Similar to thin...
Table 1. Thermal conductivity comparison for nanowire of length 2 µm.

| Diameter (nm) | Gray BTE (present work) (W/m K) | Experiments [11] (W/m K) |
|--------------|---------------------------------|--------------------------|
| 37           | 21.01                           | 17.53                    |
| 56           | 27.84                           | 25.69                    |
| 115          | 44.43                           | 40.56                    |

Figure 5. Thermal conductivity as a function of constriction ratio.

Film, thermal conductivity of unconstricted nanowire is found to be significantly smaller than the bulk. Note that for nanowire whose diameter is smaller than the mean free path, effective phonon mean free path is accepted to be equal to its diameter.[15,30] Hence, as the phonons are traveling from hot reservoir to cold reservoir in constrained nanowire, effective phonon mean free path is gradually reducing. Consequently, with increase in constriction, the total resistance offered by nanowire will increase, reducing the thermal conductivity. It is also worth noticing that irrespective of constriction ratio, thermal conductivity of nanowire is always less than that of thin film. This observation is consistent with the finding of Walkauskas et al. [32]. Quantitative explanation behind such observation is that nanowire has higher area to volume ratio; thus, phonon-boundary scattering becomes more dominant in nanowires compared to thin films.

3.2.2. Variation in temperature distribution

The effect of constriction on temperature distribution in nanostructure is also explored. Figure 6 represents the temperature distribution along the centerline of (a) thin film and, (b) nanowire for range of constriction ratio. The temperature is normalized as $\Theta = (T - T_2)/(T_1 - T_2)$ and location in $z$-direction is normalized as $z^* = z/L$. At constriction ratio of 1, linear temperature variation is observed for both thin film and nanowire. For constriction ratio less than 0.25, temperature is roughly uniform near the broad end of nanowire (i.e. $z^* = 0.8 \sim 1$), which implies nearly ballistic transport of phonon near the broad end. In contrast to transport near broad end, phonon transport near narrow end of nanowire becomes increasingly diffusive (i.e. showing linear-like temperature distribution) with increase in constriction. Thus, with increased constriction, existence of two different transport regime is observed in case of nanowire. Although, response of thin film and nanowire are similar to an extent, conclusions similar to nanowire cannot be

Figure 6. Temperature distribution for range of constriction ratio: (a) thin film and (b) nanowire.
drawn for thin film. Furthermore, with increase in constriction, temperature jump at the narrow end is found to increase. Possible reason behind such trend is that with increase in constriction, the narrow end tends to form a critical bottleneck for phonons to reach cold reservoir.

4. Summary

In this paper, the gray BTE with the relaxation-time approximation is used to study the effect of constriction on phonon transport in thin films and nanowires. It is observed that with the increase in degree of constriction, thermal conductivity of nanostructure decreases. Moreover, it is found that thin film and nanowire respond differently to constriction. For nanowire, with increased constriction, existence of two different regimes is observed. Tailoring of nanostructure property can open up exciting avenues in the area of nanoscale manufacturing, electronic device cooling and nanoscale thermometry, etc.

Disclosure statement

No potential conflict of interest was reported by the authors.

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