

Modeling nanostructure lattice thermal conductivity

The dispersion relation role

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Abstract We present an analytical model for the lattice thermal conductivity of semiconductor nanostructures, based on solving the Boltzmann transport equation in the relaxation time approximation. The improved model is then used to predict the lattice thermal conductivity of three samples of silicon nanowire (Si NW) with diameters 50, 98, and 115 nm. Derived formulas of the lattice thermal conductivity and correction term are presented, which differs from that of Callaway in that it considers the acoustic phonon dispersion relation. Combining the scattering relaxation rate for phonon–phonon, mass difference and boundary was carried out in the analysis of the experimental data and also considering the separate contributions for transverse and longitudinal phonons. The present theoretical model of lattice thermal conductivity agrees well with the available experimental data of Si NW over a wide range of temperature.

Keywords Nanostructure · Dispersion relation · Lattice thermal conductivity · Silicon nanowire

List of symbols

K	Lattice thermal conductivity
ΔK	Correction term
$g(\omega)$	Density of state
C_v	Specific heat
x	Dimensionless parameter
v_s	Phase velocity
v	Group velocity
θ_D	Debye temperature

τ_C	Combined scattering relaxation rates
τ_N	Relaxation rate of normal process
τ_U	Relaxation rate of Umklapp process
$N_q(\lambda)$	Displacement distribution function
N_q^0	Equilibrium distribution function
∇T	Temperature gradient
τ_B^{-1}	Boundary scattering relaxation rate
τ_M^{-1}	Mass difference scattering relaxation rate
τ_{3ph}^{-1}	3-Phonon scattering relaxation rate

Introduction

One-dimensional (1D) materials such as various kinds of nanowires and nanotubes have attracted considerable attention due to their potential application in electronic and energy conversion devices [1–3]. The study of lattice thermal conductivity of semiconductor nanowires plays a crucial role in the development of a new generation of thermoelectric materials [4]. It is then very clear that the theoretical prediction of the thermal conductivity of the nanowires prior to their fabrication is a desirable goal, both from the applied and basic research points of view. Thermal transport, in semiconductor nanowires, is strongly influenced by boundary scattering even at room temperature [5–7]. In rough silicon nanowires, the boundary scattering leads to a decrease in thermal conductivity with respect to bulk [5, 8], which has opened up possibilities of using this structures as efficient thermoelectric materials [9]. The reduction of nanowire thermal conductivity with respect to bulk attributed to the change in the phonon density of states and phonon boundary scattering [10]. It is now widely accepted that the thermal management in nanostructure devices becomes increasingly important as

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the size of the device reduces. Reducing the size of nanostructures [11] and surface decoration [12] have also been shown to promote boundary scattering and lead to a thermal conductivity decrease. Donadio and Galli [11] found that the computed thermal conductivity strongly depends on the surface structure. It may be as high as that of bulk Si for crystalline wires, while wires with amorphous surfaces have the smallest thermal conductivity, about 100 times lower than the bulk. Li et al. [13] measured the thermal conductivity of Si NW with diameters of 22, 37, 56, and 115 nm over a temperature range of 20–230 K. For the smaller diameter wires, the deviation from Debye T^3 law can be clearly seen at low temperature. Their results show that besides phonon boundary scattering, some other effects could play important role. In the frame of Callaway model, Mingo et al. [14, 15] attempted to calculate the Si NW thermal conductivity by omitting the normal processes, and considering, in addition to the resistive phonon mechanisms arisen from Umklapp processes, crystal imperfections scattering, and boundary scattering. The approach of Mingo employs the full phonon dispersion relation of material. Only bulk data are used as inputs for the calculation. Measurements of the effect of defects on lattice thermal conductance in the nanowire structure also showed the decrease of thermal conductance at low temperature [16]. Huang et al. [17] theoretically achieved a direct measurement of lattice thermal conductivity of a hollow Si NW under the relaxation time approximation. Their results show that the thermal conductivity is decreased markedly below the bulk value due to phonon confinement and boundary scattering.

It is well known that when the size of a bulk material reduces to the range of nanoscale. Investigation on the effects of nanoscale size dependent parameters on lattice thermal conductivity are predicted using the Debye–Callaway model including transverse and longitudinal modes for Si NW [18]. Recently Kazan et al. [19] presented a rigorous analysis of the thermal conductivity of bulk and nanowire silicon which takes into account the exact physical nature of the various acoustic and optical phonon mechanisms. They derived formalism for the lattice thermal conductivity that takes into account the phonon incidence angles. Thermal conductivity of thin Si NWs as a function of decreasing nanowire diameter shows an expected decrease due to increased surface scattering effects. The thermal conductivity data at very small diameter (<1.5 nm) shows an increasing nature, which is attributed to the phonon confinement effect [20]. Alan et al. [21] proposed a high temperature analytical model for the size dependence of thin film and nanowire thermal conductivity that requires no fitting parameter. They compared the predictions and experimental measurements on silicon structures.

Previously, an approximate method was developed by Callaway [22] to obtain an expression for the lattice thermal conductivity at low temperatures. Several approximations have been assumed to get this formula, which can be summarized as follows: (1) The Debye model has been used, which represents a simple linear dispersion relation for each branch of the phonon spectrum (this is the limiting form for small wave vector in real crystals). Consequently, he has employed the group velocity to be equal to the phase velocity. (2) It is assumed that the deviation from equilibrium is small, so he has replaced the phonon distribution function by equilibrium one. (3) Making no distinction between the contributions due to transverse and longitudinal phonons. Ever since, it has been widely used for the interpretation and analysis of thermal conductivity data in different classes of materials [14, 18, 21, 23–26]. A great deal of effort has been devoted to modifying Callaway model [27–29].

Here, we propose a theoretical model for calculating the lattice thermal conductivity and the correction term in nanostructure materials. They are based on the solution of phonon Boltzmann transport equation, which takes into account the role of the dispersion relation. To test the applicability of the expressions proposed, the lattice thermal conductivity of Si NWs with diameters of 50, 98, and 115 nm are calculated between temperatures of 2 and 350 K, and comparing them with that of the experimental data, with detailed exposition to the role of the physical parameters. Conclusions are reported in the last section. In addition to the three-phonon scattering, we consider other phonon scattering such as boundary and point defect.

Theory

Theoretical background

It is well known that the lattice thermal conductivity is represented by

$$K = \frac{1}{3} \sum_{\vec{q}} C_{v_i}(\omega_{\vec{q}}) \tau_i(\vec{q}) v_i^2. \quad (1)$$

The average energy of a mode in thermal equilibrium is found by summing all possible energy value each weighted by the probability of its occurrence, and the total vibration energy for a solid at temperature T is summed over all normal modes. Since all solids have large number of normal modes, the spectrum can be treated as continuous, so the total energy is

$$E_T = \sum_i \frac{\hbar\omega}{(e^{\hbar\omega/K_B T} - 1)} g(\omega) d\omega \quad (2)$$

and the specific heat per normal mode for frequency ω is

$$C_{v_i}(\omega) = \frac{\hbar^2}{K_B T^2} \int_0^{\omega_m} H(\omega)g(\omega)d\omega. \tag{3}$$

Then Eq. (1) has the form

$$K = \frac{\hbar^2}{3K_B T^2} \sum_i \int_0^{\omega_m} \tau(\vec{q}, i)v^2(\vec{q}, i)\omega^2 H(\omega)g(\omega)d\omega, \tag{4}$$

where

$$H(\omega) = e^{(\hbar\omega/K_B T)}(e^{\hbar\omega/K_B T} - 1)^{-2} \tag{5}$$

and $g(\omega)d\omega$ represents the density of phonon states,

$$g(\omega)d\omega = \frac{NV}{2\pi^2} q^2 dq. \tag{6}$$

Here, N and V are number and volume of the primitive cell, respectively.

Model development

Lattice thermal conductivity

Consider a one-dimensional monatomic lattice with a lattice constant a in which forces are assumed to act between one atom and its first nearest neighbors. The possible angular frequencies of the modes in which all atoms vibrate with the same frequency vary with wave vector according to the relation [30].

$$\omega = \omega_m \sin(\bar{q}a/2). \tag{7}$$

Thus $g(\omega)d\omega$ can be expressed as

$$g(\omega)d\omega = \frac{4V_0(\sin^{-1}(\omega/\omega_m))^2 d\omega}{\pi^2 a^3 \omega_m \sqrt{1 - (\omega/\omega_m)^2}}. \tag{8}$$

Thus, the phase and group velocities can be written as

$$v_s = \frac{a\omega}{2 \sin^{-1}(\omega/\omega_m)} \tag{9}$$

$$v = \frac{a\omega_m}{2} \sqrt{1 - (\omega/\omega_m)^2}. \tag{10}$$

The lattice thermal conductivity per unit volume reduces to

$$K_i = c\theta_i \int_0^{\theta_i/t} \tau_{c,i}x^2 Q_i(x)F_i(x)M_i^2(x)dx, \tag{11}$$

where

$$c = (K_B^3 T/3\pi^2 a\hbar^2), \tag{12}$$

$$\theta_i = \hbar\omega_{im}/K_B, \tag{13}$$

$$Q_i(x) = e^x(e^x - 1)^{-2}, \tag{14}$$

$$x = \hbar\omega/K_B T, \tag{15}$$

$$F_i(x) = \sqrt{1 - (Tx/\theta_i)^2}, \tag{16}$$

and

$$M_i(x) = (\sin^{-1}(Tx/\theta_i)) \tag{17}$$

where the θ 's are the temperature relating to the Brillouin zone boundary in the i th branch and $\tau_{c,i}$ are the combined scattering relaxation time. Taking into account the three types of polarization modes, the lattice thermal conductivity is then given by

$$K = 2K_T + K_L \tag{18}$$

Correction term ΔK

All phonon scattering processes have a direct effect on thermal conductivity by restoring a non-equilibrium distribution to equilibrium situation. The normal processes play a special role in the estimation of thermal conductivity, since they are the only Momentum-conserving scattering processes, which are not tend to restore the equilibrium phonon distribution, and they cannot cause thermal resistance by themselves. On the other hand, due to the fact that they exchange energy between modes, normal processes influence the other scattering processes.

Callaway [22] assumed that normal processes restore an arbitrary phonon distribution (representing a heat flow) to the displaced distribution function, which in turn corresponds to the same heat flow but is no longer changed by normal processes. The relaxation time for such processes is τ_N and the relaxation time for processes which restore the equilibrium distribution function is τ_U . The total rate of change of $N(q)$ is then expressed as

$$\left(\frac{\partial N_q}{\partial t}\right)_{\text{scatt.}} = \frac{N_q(\vec{\lambda}) - N_q}{\tau_N} + \frac{N_q^0 - N_q}{\tau_U}, \tag{19}$$

where $\vec{\lambda}$ is an arbitrary constant vector in the direction of temperature gradient and $N_q(\vec{\lambda})$, displaced distribution function, is given by

$$N_q(\vec{\lambda}) = \left(\exp\left(\frac{\hbar\omega - \vec{q}\cdot\vec{\lambda}}{K_B T}\right) - 1\right)^{-1}. \tag{20}$$

To first order in $\vec{\lambda}$, when $\hbar\vec{q}\cdot\vec{\lambda}/K_B T$ is small, $N_q(\vec{\lambda})$ can be written as

$$N_q(\vec{\lambda}) \approx N_q^0 + \frac{\vec{\lambda}\cdot\vec{q}}{K_B T} H(\omega). \tag{21}$$

When a steady state has been established using Eqs. (19) and (21), so the Boltzmann transport equation

$$\left(\frac{\vec{\lambda} \cdot \vec{q}}{\tau_N} - \frac{\hbar\omega}{T} \vec{v} \cdot \vec{\nabla} T \right) \frac{Q(x)}{K_B T} - \frac{n_q}{\tau_c} = 0. \quad (22)$$

Here, and $n = N - N^0$ and the combined relaxation time τ_c is $\tau_c^{-1} = \tau_N^{-1} + \tau_U^{-1}$.

Callaway [22] defines a total relaxation time τ by writing n_q as

$$n_q = -\tau \vec{v} \cdot \vec{\nabla} T \frac{\hbar\omega}{K_B T^2} Q(x). \quad (24)$$

Now it is desired to determine τ (the total relaxation time) in terms of τ_c and τ_N . After substituting Eqs. (23) and (24) into (22), we get

$$\left(\frac{\tau}{\tau_c} - 1 \right) \frac{\hbar\omega}{K_B T} \vec{v} \cdot \vec{\nabla} T + \frac{\vec{\lambda} \cdot \vec{q}}{\tau_N} = 0. \quad (25)$$

In an isotropic medium, $\vec{\lambda} \propto \nabla T$ so it is convenient to introduce another parameter β which has the dimension of a relaxation time by defining

$$\vec{\lambda} = -\hbar\beta v_s \nabla T / T. \quad (26)$$

On using

$$\vec{q} = \vec{v}_s \omega / v_s^2 \quad (27)$$

$$\vec{\lambda} \cdot \vec{q} = -\frac{\hbar\omega}{v_s} \beta v \vec{v}_s \cdot (\vec{\nabla} T / T). \quad (28)$$

Accordingly, Eq. (25) simplified to

$$\tau = \tau_c (1 + (\beta v / v_s \tau_N)). \quad (29)$$

The constant β is determined by recalling that the normal processes conserve momentum. This condition is

$$\int \left(\frac{\partial N_q}{\partial t} \right) q d^3 q = \int \frac{N(\vec{\lambda}) - N}{\tau_N} q d^3 q = 0. \quad (30)$$

Using the value of $N(\vec{\lambda})$ [Eq. (21)], we can then write Eq. (30)

$$\int \left[\frac{-n}{\tau_N} + \frac{\vec{\lambda} \cdot \vec{q}}{\tau_N K_B T} Q(x) \right] q d^3 q = 0. \quad (31)$$

Following the substitution of Eqs. (24) and (28), the integral has the form

$$\int Q(x) \left[\frac{x}{T} \vec{v} \cdot \vec{\nabla} T \left(\tau - \frac{v\beta}{v_s} \right) \right] \frac{q}{\tau_N} d^3 q = 0. \quad (32)$$

The value of $q d^3 q$ can be determined from the dispersion relation [Eq. (30)] in terms of the variables x and θ , as

$$q d^3 q = \frac{64\pi T M^3(x)}{a^4 \theta} F(x) dx. \quad (33)$$

Hence, with the help of Eqs. (10) and (33), Eq. (32) modified to

$$\int_0^{\theta/T} x Q(x) M^3(x) \frac{(\tau - v\beta/v_s)}{\tau_N} dx = 0. \quad (34)$$

From Eqs. (9) and (10) we denote to the ratio v/v_s as,

$$\frac{v}{v_s} = \frac{\theta}{Tx} F(x) M(x). \quad (35)$$

On using Eq. (29) for τ , Eq. (35) for v/v_s and the integral of Eq. (34), we have

$$\beta = I_1 / \frac{\theta}{T} I_2, \quad (36)$$

where

$$I_1 = \int_0^{\theta/T} \frac{\tau_c}{\tau_N} x Q(x) M^3(x) dx. \quad (37)$$

$$I_2 = \int_0^{\theta/T} \left[\frac{1}{\tau_N} \left(1 - \frac{\tau_c}{\tau_N} \right) Q(x) F(x) M^4(x) \right] dx. \quad (38)$$

Substitute Eq. (35) in Eq. (29), we can write τ as

$$\tau = \tau_c \left[1 + \frac{\beta\theta}{\tau_N T x} F(x) M(x) \right]. \quad (39)$$

Recall the value of β from Eq. (37), the lattice thermal conductivity (Eq. 7) can be rewritten as

$$K_i = [c\theta_i I_3 + \Delta K], \quad (40)$$

$$\Delta K = c\theta_i I_1 I_4 / I_2, \quad (41)$$

$$I_3 = \int_0^{\theta_i/T} [\tau_c x^2 Q(x) F(x) M^2(x)] dx, \text{ and} \quad (42)$$

$$I_4 = \int_0^{\theta_i/T} \left[\frac{\tau_c}{\tau_N} x Q(x) F^2(x) M^3(x) \right] dx, \quad (43)$$

where ΔK is known as the correction term due to the three-phonon normal processes.

Phonon relaxation rates

In our model, we consider acoustic phonon relaxation in resistive processes, such as three-phonon normal and Umklapp scattering, mass difference scattering (isotopes and impurity), and boundary scattering. The combined scattering relaxation rates can be obtained by the summation of the inverse relaxation time for these scattering processes and in our case it is given as

$$\tau_{c,i}^{-1} = \tau_{3ph,i}^{-1} + \tau_{M,i}^{-1} + \tau_{B,i}^{-1} \tag{44}$$

The Normal processes (N) for longitudinal (L) and transverse phonons (T) are fixed as [31]

$$\tau_{N,T}^{-1} = B_{N,T} \omega T^4 \tag{45}$$

$$\tau_{N,L}^{-1} = B_{N,L} \omega^2 T^3, \tag{46}$$

While Klemens [32] has suggested the form of Umklapp (U) processes as

$$\text{gathered } \tau_{U,T}^{-1} = B_{U,T} \omega T^3 e^{-\theta_{D,T}/\alpha T} \tag{47}$$

$$\tau_{U,L}^{-1} = B_{U,L} \omega^2 T^3 e^{-\theta_{D,L}/\alpha T}. \tag{48}$$

Impurity scattering process contributes greatly to the lattice thermal conductivity at low temperatures. The relaxation rate for mass difference scattering is calculated using a simple model by Klemens [32]:

$$\tau_M^{-1} = A\omega^4, \tag{49}$$

where A is the scattering strength parameter.

The important scattering process at low temperature is that due to the boundary of the solid. The consequence of this were seen by Casimir [33] who treated the flow of the phonons as analogous to the flow of the radiation down a tube having diffusive scattering walls (Theory of black body radiation). It is also pointed out that the important phonon wavelength, even at the lowest temperatures, would be small compared with the roughness of the surface. As a result the boundary scattering relaxation rate is given by the ratio of the velocity to the characteristic length of the specimen which is called Casimir length. Thus, the inverse relaxation time due to boundary scattering of phonon is

$$\tau_B^{-1} = v/d, \tag{50}$$

where d is the effective diameter of the sample. The scattering strengths $B_{N,i}$, $B_{U,i}$, A_i , and $\tau_{B,i}^{-1}$ are treated as adjustable parameters.

Results and discussion

The theoretical $K(T)$ curves for three samples of Si NW obtained with our model are measured in the temperature range 2–350 K, and plotted in Fig. 1 using solid lines. The Hochbaum et al. [6] experimental data of Si NWs with diameters of 50, 98, and 115 nm at a temperature range of 20–320 K have also been shown by comparison. The values of $\theta_{D,i}$ and v_i are obtained from Kazan et al. [19]. By adjustment of the scattering strengths (Table 1), the total thermal conductivity of Si NW has been calculated with the help of Eqs. (40) and (44). The percentage deviation in the thermal conductivity is given as %Deviation =

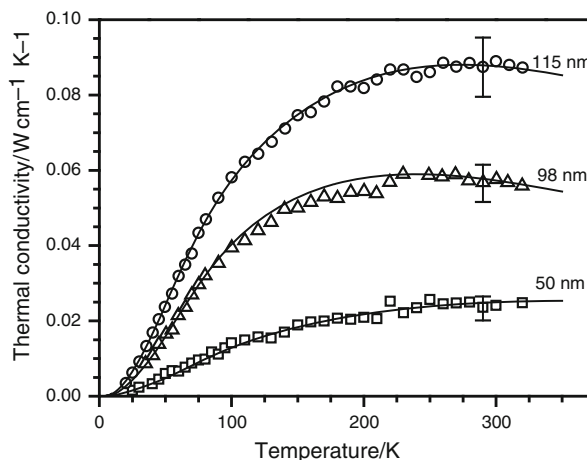


Fig. 1 Temperature dependence of lattice thermal conductivity for Si NW. Lines are the present theoretical results and symbols are the experimental data

Table 1 Values of parameters used in the present calculation

Parameter	Sample L/nm		
	50	98	115
$\tau_{B,T}^{-1} (s^{-1}) 10^{12}$	4.8	2.3	0.7
$\tau_{B,L}^{-1} (s^{-1}) 10^{12}$	1.5	1.5	1.5
$\tau_{M,T}^{-1} (s^3) 10^{-38}$	30	5.5	4.7
$\tau_{M,L}^{-1} (s^3) 10^{-38}$	10	4.5	4.5
$\tau_{N,T}^{-1} (K^{-4}) 10^{-10}$	5.0	2.5	2.0
$\tau_{U,T}^{-1} (K^{-3}) 10^{-6}$	6.9	4.85	2.83
$\tau_{N,L}^{-1} (s.K^{-3}) 10^{-18}$	6.0	6.0	6.0
$\tau_{U,L}^{-1} (s.K^{-3}) 10^{-16}$	7.5	6.5	5.5

$|\frac{K_{Exp.} - K_{Theo.}}{K_{Exp.}}| \times 100\%$. The temperature variation of % Deviation for the three samples is compared in Fig. 2.

The separate percentage contributions of the transverse and longitudinal phonons to the total lattice thermal conductivity can be studied with the help of Fig. 3. Figures 4 and 5 show the variation with temperature of ΔK and % ΔK ($\Delta K/K \times 100$) to the total lattice thermal conductivity, respectively. The percentage contributions of the three-phonon normal and Umklapp processes to τ_{3ph}^{-1} have also been studied for both modes of phonons and are illustrated in Figs. 6 and 7.

As we mentioned earlier, Callaway [22] obtained the integral expression through various assumptions and approximations, which appears to be a reasonable first step in obtaining qualitative fit to thermal conductivity data only at low temperature [27]. This is undoubtedly attributed to the fact that Callaway’s form was expressed in terms of Debye approximation, which is far from reality. It is

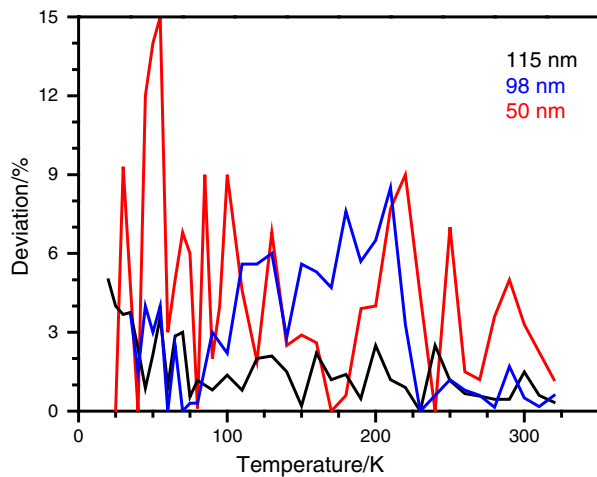


Fig. 2 Temperature variation of the %Deviation in the thermal conductivity

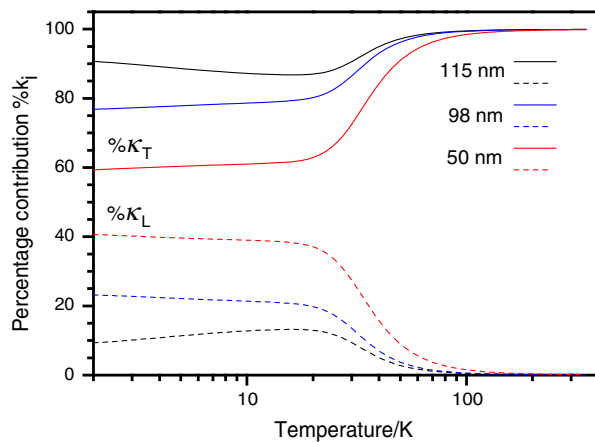


Fig. 3 Percentage contributions of transverse and longitudinal phonons for Si NWs

interesting to note that the Debye picture is a good representation up to approximately 60 % of the full acoustic phonon spectrum [34]. We feel that the importance of this work lies in obtaining a form that is a characteristic of the crystal. The new feature that we added to the expression of the lattice thermal conductivity are using the exactly acoustic phonon dispersion, which are the basic approximations suggested by Callaway. Thus, a formulation of the type presented here would eliminate these assumptions and approximations in the analysis of the lattice thermal conductivity.

Figures 1 and 2 clearly demonstrate a fairly good quantitative agreement between the predicted and observed lattice thermal conductivity of the sample. This agreement adds support to the wide scope and applicability of the model proposed, and one can conclude that the new

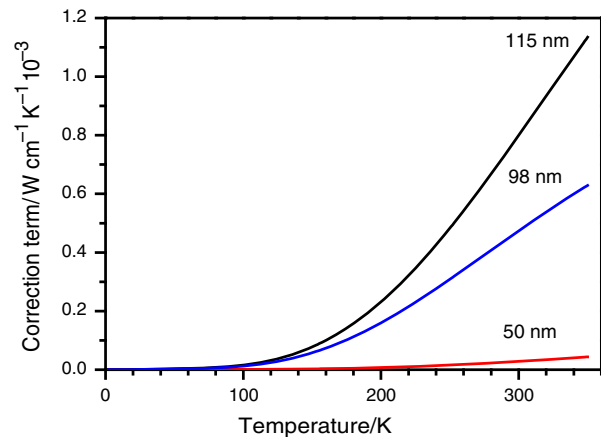


Fig. 4 Temperature dependence of the correction term of Si NWs

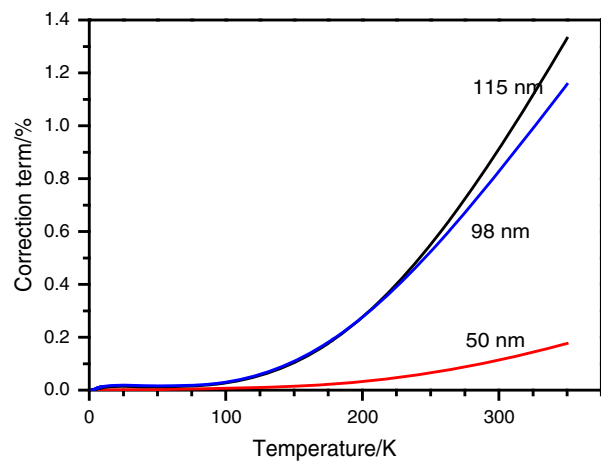


Fig. 5 Percentage contribution of the correction term to the overall lattice thermal conductivity of Si NWs

proposed expressions are successfully employed to explain the temperature dependence of the lattice thermal conductivity of Si NW. A very slight departure of the calculated values from the experimental one is observed.

With the help of Fig. 3, it can be concluded that most of the heat transport by the transverse phonons alone is relevant to the earlier findings [35–38]; it can be confirmed that the percentage contribution of transverse phonon increases with temperature, meanwhile the opposite is true for the longitudinal phonons.

By examining the curves in Figs. 4 and 5, it can be confirmed that the maximum values of the correction term ranged from $4.39 \cdot 10^{-5}$ to $1.13 \cdot 10^{-3}$, which reflects that the maximum values for $\% \delta K$ change from $\%0.17$ for 50 nm to $\%1.33$ for the 115 nm wire diameter. As shown in these figures, the correction term is very small compared to the lattice thermal conductivity of Si NW. The lower values of the correction term can be explained by the fact that at low

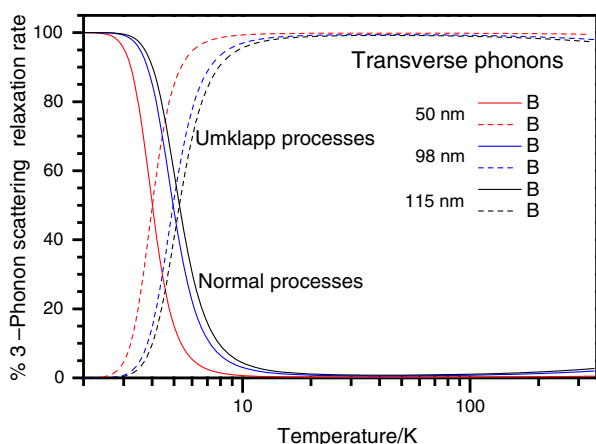


Fig. 6 The percentage contributions of the $\tau_{3ph,N}^{-1}$ and $\tau_{3ph,U}^{-1}$ processes toward the τ_{3ph}^{-1} for transverse phonons of Si NWs

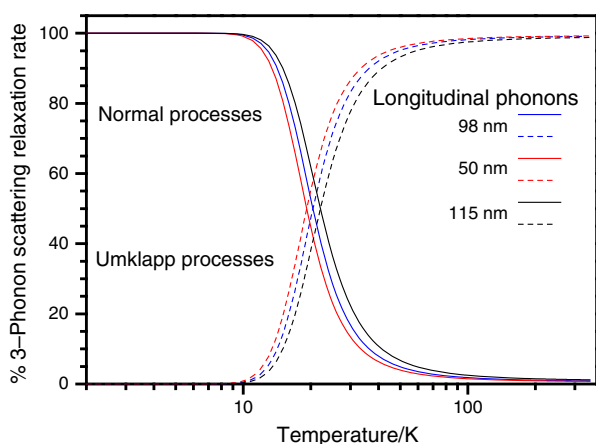


Fig. 7 The percentage contributions of the $\tau_{3ph,N}^{-1}$ and $\tau_{3ph,U}^{-1}$ processes toward the τ_{3ph}^{-1} for longitudinal phonons of Si NWs

temperatures, the contribution of $\tau_{3ph,N}^{-1}$ is less than the other scattering relaxation rates. It is worth noting that in our calculations, we have used the full lattice thermal conductivity expression (Eq. 40).

Close inspection of Figs. 6 and 7 clearly indicates that at low temperatures, τ_N^{-1} dominates over τ_U^{-1} below certain temperature (which varies according to the diameter), and the opposite is true above that temperature. In other words, τ_N^{-1} decreases with increasing temperature, an opposite trend is shown for τ_U^{-1} . Meanwhile, one can conclude that at low temperatures, the most of the heat is transported by phonons, which conserve momentum, while at high temperatures, the role of those phonon processes, which do not conserve momentum in the lattice thermal conductivity, becomes predominant. Previous workers [35, 38–40] find similar results.

The important scattering process at low temperature is that due to the boundary of the solid, including crystallite boundaries for polycrystalline materials. The consequence of this were seen by Casimir [33] who calculated the equivalent mean free path as $L = D$ for a cylindrical specimen with diameter D and $L = 1.12b$ for a square shape specimen with edge length b . However, it is also pointed out that the important phonon wavelength, even at the lowest temperatures, would be small compared with the roughness of the surface. As a result, the boundary scattering relaxation rate is given by the ratio of the velocity to the characteristic length of the specimen which is called Casimir length (L) ($\tau_B^{-1} = v/FL$). F (Correction factor) related to the phonon specularity and should be equal to one for completely diffused scattering and large than unity if part of the phonons are specularly reflected. Whenever partial specular reflection occurs, F takes values between zero and one. One of the reasons for $F < 1$ could be the finite length of the sample and/or the existence of the internal boundaries due to the microscope fluctuations in the composition of the compound [41]. Thus, F is related to the degree of specularity of the boundary scattering. The boundary scattering rate is the only one that directly depends on the diameter of the wire $\tau_B^{-1} = v/FD$. The phonon mean free path approaches $\approx FD$ if the boundary scattering dominates over other mechanisms. For above reason, we will show our results in term of $d = FD$, rather than D . For the transverse branch, the effective Si NW diameters are 1.14, 2.42, and 8.22 nm, and 5.23, 5.414, and 5.48 for longitudinal branch, corresponding to the experimental one 50, 98, and 115 nm, implying $F \approx 0.022, 0.024, \text{ and } 0.07$, respectively, while for longitudinal branch $F \approx 0.104, 0.055, \text{ and } 0.047$, respectively. The decrease in lattice thermal conductivity for rough Si NWs reported by Hochbaum et al. [6] clearly indicates that the boundary scattering in the Si nanowire initially measured by Li et al. [13] and modeled by Mingo et al. [14, 15] was far from completely diffusive and the corresponding F value should be below one.

Conclusions

In summary, this paper presents the resolution of Boltzmann transport equation to establish formalism for the lattice thermal conductivity of nanostructure materials that takes into account the role of phonons dispersion relation. A model of the type presented here would eliminate Callaway assumptions and approximations in the analysis of the lattice thermal conductivity. The analysis presented here has the advantage that it is, in principle, a simple extension of the existing theories and that it is physically quite plausible. Phonon dispersion relation modification leads to significant

effects on the lattice thermal conductivity formula. The temperature dependence of lattice thermal conductivity for the Si NW diameters 50, 98, and 115 nm indicates that the model used in the present calculation is perfectly applicable in the full temperature range (2–350 K). We have measured the correction term, the effective diameters, and the degree of specularity of the boundary scattering. The surface specularity of the samples studied appears to be rather low, suggesting that partial specular reflection occurs. The contribution of the correction term toward the total lattice thermal conductivity is found to be small and can be ignored in the calculation of the lattice thermal conductivity of the samples under consideration. The present calculation further establishes that transverse phonons make a major contribution toward the lattice thermal conductivity of Si nanowire. The dependence of the three-phonon scattering on the normal processes becomes more pronounced as the temperature decreases, while the Umklapp processes do so as the temperature increases.

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