Carrier concentration effect and other structure-related parameters on lattice thermal conductivity of Si nanowires

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Abstract. Lattice thermal conductivity (LTC) of Si bulk and nanowires (NWs) with diameter 22, 37, 50, 56, 98 and 115 nm was investigated in the temperature range 3–300 K using a modified Callaway model that contains both longitudinal and transverse modes. Using proper equations, mean bond length, lattice parameter, unit cell volume, mass density, melting temperature, longitudinal and transverse Debye temperature and group velocity for all transverse and longitudinal modes were calculated for each NW diameter mentioned. Surface roughness, Gruneisen parameter and impurity were used as adjustable parameters to fit theoretical results with experimental curves. In addition, values of electron concentration and dislocation density were determined. There are some phonon scattering mechanisms assumed, which are Umklapp and normal processes, imperfections, phonon confinement, NW boundaries, electrons scattering and dislocation. Dislocation density less than 10^{14} m^{-2} for NWs and 10^{12} m^{-2} for bulk has no effect on LTC. Also, electron concentration less than 10^{22} m^{-3} for NWs and 10^{16} m^{-3} for the bulk has no effect. On increasing dislocation density and electron concentration, LTC comparably decreases.

Keywords. Lattice thermal conductivity; Si nanowire; dislocation density; conduction electrons.

1. Introduction

Heat conduction is a fundamental property of solids, which is due to transfer of phonons across a material when a temperature gradient occurs. This feature attracts significant interest, particularly for designing electronic devices. Miniaturization of electronic chips, based on Moore's prediction [1], makes lattice thermal conductivity (LTC) an important problem for researchers all around the world. There are many experimental and theoretical investigations for reducing size of semiconductor nanowires (NWs). Silicon NWs are used as solar cells and nanoelectronics power sources [2]; apart from these, they are used to prepare high-resolution atomic force microscopes (AFMs) [3].

Precise information and quantitative calculations of the Si NWs thermal conductivity at both low and high temperatures are essential to understand their thermal effects.

LTC has a significant decrease in NWs in relation to its bulk value. There are theoretical [4,5] and experimental investigations [6,7] on this. Single-crystalline intrinsic Si NWs with diameters of 22, 37, 56 and 115 nm were measured using a microfabricated suspended device over a temperature range of 20–320 K [6], and enhanced thermoelectric performances of rough silicon NWs for 115, 98 and 50 nm were considered [7].

Li *et al* [6] and Hochbaum *et al* [7] reported experimental results for LTC of Si NWs based on the Boltzmann transport equation approach, clearly assuming a variation in

the nonequilibrium phonon distribution for purely diffuse scattering from wire boundaries when the structure of NWs is assumed to be similar to that of the bulk. For GaN, Zou [8] showed that decreasing LTC is, in addition to point defect scattering, phonon confinement and boundary scattering, affected by change in the nonequilibrium phonon distribution, causing scattering diffusion at the surface of NWs.

Mingo [9] and Yang *et al* [10] studied NWs coated by an amorphous material for simple and real Si NWs. They presented a useful way to survey LTC of NWs coated with an amorphous material. On the other hand, Yang *et al* [10] concluded that the effective thermal conductivity of two-dimensional Si–Ge nanocomposites decreases as the radius of NW inclusion decreases because of the relative increase in boundary scattering area per unit volume. In addition, LTC for Si was calculated through a Monte Carlo model as a solution of the Boltzmann transport equation, where phonon group velocity, phonon confinement and three-phonon interaction were assumed [11]. The same simulation was used to calculate LTC in Ref. [12], with good agreements for considered diameters.

In the present work we investigated the theoretical LTC for Si NWs and correlated with experimental data reported by [6,7]. We want to investigate numerically the effect of each phonon–electron and phonon–dislocation scattering on Si bulk and likewise on Si NWs. We improve the work of Omar and Taha [13], who investigated some other parameters

such as phonon–phonon Umklapp scattering, mass difference scattering, boundary scattering and normal three-phonon scattering. Furthermore, mean free path (MFP), Gruneisen parameter and surface roughness were used as adjustable parameters for fitting curves.

2. Theory and calculations

2.1 Callaway model

There are many carriers for transferring heat; however, in semiconductor materials frequently heat transfer is by acoustic phonons [8], since the value of optical phonon velocity is smaller than group velocity. Analytical thermal conductivity models are typically developed based on the Boltzmann transport equation and under the single-mode relaxation time approximation [14], which is called Callaway's phenomenological theory [15]. The Callaway theory includes all relaxation times of the phonon scattering process. The LTC formula [5] is as follows:

$$\kappa = AT^3 \int_0^{\theta_D/T} \tau_C J(x) dx, \quad (1)$$

where $A = (k_B/\hbar)^3 (k_B/(2\pi^2 v))$, $J(x) = x^4 e^x (e^x - 1)^{-2}$, $x = \hbar\omega/k_B T$, k_B and $\hbar$ are the Boltzmann and reduced Planck constants, respectively, v is phonon group velocity, ω is the phonon angular frequency, θ_D is Debye temperature, T is the absolute temperature and τ_C is the total (combined) phonon relaxation time.

Equation (1) is the theoretical estimation formula for thermal conductivity of bulk, which is known as the Callaway formula. Thus, this model assumes a Debye-like phonon spectrum with no anisotropies or specific structures in the phonon density of states. This equation can be used for calculating LTC of NWs and thin films [4,16] as well. Zou [8] and Balandin and Wang [4] considered deviation of the nonequilibrium phonon distribution from its bulk value due to diffuse boundary scattering at the wire surface to calculate thermal conductivity for Si NWs. Morelli *et al* [17] and Asen-Palmer *et al* [18] modified the Debye–Callaway model, by considering normal three-phonon processes and both transverse and longitudinal phonons explicitly, which is confirmed in this work. The LTC involves two terms $\kappa = \kappa_L + \kappa_T$, where κ_L and κ_T are given as follows [17,18]:

$$\kappa = \kappa_L + 2\kappa_T, \quad (2)$$

$$\kappa_L = \kappa_{L1} + \kappa_{L2}, \quad (2)$$

$$\kappa_T = \kappa_{T1} + \kappa_{T2}. \quad (3)$$

The partial conductivities κ_{L1} and κ_{L2} are the usual Debye–Callaway terms given by

$$\kappa_{L1} = \frac{1}{3} A_L T^3 \int_0^{\theta_D^L/T} \tau_C^L(x) J(x) dx, \quad (4)$$

$$\begin{aligned} \kappa_{L2} = & \frac{1}{3} A_L T^3 \left[\int_0^{\theta_D^L/T} \frac{\tau_C^L(x)}{\tau_N^L(x)} J(x) dx \right]^2 \\ & \times \left[\int_0^{\theta_D^L/T} \frac{\tau_C^L(x)}{\tau_N^L(x) \tau_R^L(x)} J(x) dx \right]^{-1}, \end{aligned} \quad (5)$$

and likewise, for the transverse phonons

$$\kappa_{T1} = \frac{1}{3} A_T T^3 \int_0^{\theta_D^T/T} \tau_C^T(x) J(x) dx, \quad (6)$$

$$\begin{aligned} \kappa_{T2} = & \frac{1}{3} A_T T^3 \left[\int_0^{\theta_D^T/T} \frac{\tau_C^T(x)}{\tau_N^T(x)} J(x) dx \right]^2 \\ & \times \left[\int_0^{\theta_D^T/T} \frac{\tau_C^T(x)}{\tau_N^T(x) \tau_R^T(x)} J(x) dx \right]^{-1}, \end{aligned} \quad (7)$$

where T and L in the superscripts of the above equations indicate the transverse and longitudinal phonons, respectively. In addition, θ_D^T and θ_D^L are the transverse and longitudinal Debye temperature, respectively; also

$$A_{T(L)} = \left(\frac{k_B}{\hbar} \right)^3 \frac{k_B}{2\pi^2 v_{T(L)}}, \quad (8)$$

where $v_{T(L)}$ is the transverse (longitudinal) acoustic phonon group velocity.

2.2 Phonon-scattering rates

There are different phonon scattering processes that affect the LTC in semiconductor materials. In this work, phonon–phonon (normal scattering and Umklapp processes), phonon–impurity, phonon–boundary, phonon–dislocation and phonon–electron scattering rates are taken into account. The related equations and details of these mentioned scattering rates are given as follows.

2.2a Three-phonon Umklapp and normal scattering processes: There are two types of phonon scattering in lattices, which are called as resistive. They are normal and Umklapp processes [19], in which for each longitudinal and transverse relaxation, the three-phonon Umklapp scattering rate is given by [17]

$$\left[\tau_U^{L(T)} \right]^{-1} = B_U^{L(T)} \left(\frac{k_B}{\hbar} \right)^2 x^2 T^3 e^{-(\theta_D^{L(T)}/3T)}, \quad (9)$$

where $B_U^{L(T)}$ is the Umklapp parameter strength for longitudinal (transverse) relaxation, and it can be quantitatively

Table 1. The fitting parameters of Si NWs used in this work for calculating LTC for each diameter.

r (nm)	N_{imp} (m^{-3})	N_D (m^{-2})	n_e (m^{-3})	ε	L_C (nm)	L (μm)	γ_L	γ_T
22	5.0×10^{25}	2×10^{15}	3×10^{24}	0.01000	22	4	0.3	0.100
37	9.0×10^{24}	1×10^{15}	3×10^{22}	0.36500	37	4	1.6	1.500
50	1.3×10^{27}	5×10^{15}	5×10^{24}	0	50	4	0.2	0.100
56	9.5×10^{24}	5×10^{14}	9×10^{21}	0.46700	56	4	1.4	1.200
98	4.6×10^{26}	5×10^{14}	1×10^{24}	0	98	4	0.2	0.100
115	1.0×10^{25}	1×10^{14}	9×10^{21}	0.47541	115	4	1.0	0.900
115	2.6×10^{26}	4×10^{14}	5×10^{23}	0	115	4	0.2	0.100
Bulk	1.0×10^{22}	1×10^{12}	1×10^{16}				4.0	0.385

Table 2. Calculated diameter dependence values for mean path length, Eq. (22), lattice parameter, Eq. (23), unit cell volume, Eq. (24), mass density, Eq. (25), melting temperature, Eq. (26), longitudinal and transverse Debye temperature, Eq. (28), and longitudinal and transverse phonon group velocity, Eq. (29).

r (nm)	d_{mean} ($\text{\AA}$)	α ($\text{\AA}$)	V ($\text{\AA}^3$)	ρ (kg m^{-3})	T_m (K)	θ_D^L (K)	θ_D^T (K)	v_L (m s^{-1})	v_T (m s^{-1})
22	2.3902	5.5200	21.0246	2282.61	1611.60	558.816	228.867	8084.71	5578.62
37	2.3737	5.4817	20.5905	2282.61	1644.21	570.124	233.498	8248.31	5691.51
50	2.3674	5.4674	20.4289	2300.66	1656.35	574.332	235.221	8309.19	5733.52
56	2.3656	5.4630	20.3801	2306.18	1660.02	575.604	235.742	8327.59	5746.21
98	2.3589	5.4475	20.2073	2325.90	1672.99	580.103	237.585	8392.69	5791.13
115	2.3575	5.4445	20.1735	2329.79	1675.53	580.983	237.945	8405.41	5799.91
Bulk	2.3500 ^a	5.4271	19.9807	2352.26	1685.00 ^b	586.00 ^c	240.00 ^c	8478.00 ^c	5850.00 ^c

^aRef. [22], ^bRef. [23] and ^cRef. [13].

obtained by

$$B_U^{L(T)} = \frac{\hbar \gamma_{L(T)}^2}{M v_{L(T)}^2 \theta_D^{L(T)}},$$

where $\gamma_{L(T)}$ is the longitudinal (transverse) Gruneisen parameter, which is used as an adjustable parameter to fit the curves [17]; the value for Si bulk and NWs is found and presented in table 1; here, M is the average atomic mass, which is equal to 28.0855 amu; $v_{L(T)}$ and $\theta_{L(T)}$ are longitudinal (transverse) group velocity and Debye temperature, respectively, which are calculated and recorded in table 2.

Hence, normal phonon scattering is not a resistive process [13], but it can have a significant role in determining the peak of LTC [20]. N-processes for longitudinal and transverse phonon relaxation rates, which are modified by Herring [21] and Morelli *et al* [17], are as follows:

$$\left[\tau_N^{L(T)}(\omega) \right]^{-1} = B_N^{L(T)} \omega^2 T^3, \quad (10)$$

with

$$B_N^L = \frac{k_B^3 v_L^2 V}{M \hbar^3 v_L^5} \quad \text{and} \quad B_N^T = \frac{k_B^4 v_T^2 V}{M \hbar^3 v_T^5},$$

where V , the unit cell volume, is calculated for each case and inserted in table 2.

2.2b Phonon–impurity scattering rate: Mass-difference scattering is a process that occurs because of the presence of atoms with a different mass. The different mass is due to isotopes of impurity atoms or a particular element. The NW samples contain impurities, defects and dislocations.

There are two types of point defects assumed, which are impurity and isotope atoms. To calculate the relaxation rate in term of a unit-less parameter, x , the following equation can be used [24]:

$$\left[\tau_M^{L(T)} \right]^{-1} = \left(I_{\text{iso}}^{L(T)} + I_{\text{imp}}^{L(T)} \right) \omega^4, \quad (11)$$

with

$$I_{\text{iso}}^{L(T)} = \frac{V \Gamma}{4 \pi v_{L(T)}^3} \quad \text{and} \quad I_{\text{imp}}^{L(T)} = \frac{3 V^2 S^2}{\pi v_{L(T)}^3} N_{\text{imp}},$$

where $I_{\text{iso}}^{L(T)}$ is the phonon scattering distribution due to different isotopes in the element or compound for longitudinal (transverse) modes, and $I_{\text{imp}}^{L(T)}$ is the phonon scattering distribution due to impurity; S is the scattering factor; in general its value is equal to one [24]; N_{imp} is the concentration of

Table 3. Material parameters of silicon.

Ideal gas constant	R	$8.314 \text{ (J K}^{-1} \text{ mol}^{-1})$	Ref. [23]
First surface layer height	h	0.3368 (nm)	Ref. [23]
First surface layer height	h	0.3358 (nm)	From Eq. (18)
Enthalpy of fusion	H_m	$49.819 \text{ (J mol}^{-1})$	From Eq. (20)
Bulk overall melting entropy	$S_m(\infty)$	$29.47 \times 10^{-3} \text{ (J K}^{-1} \text{ mol}^{-1})$	From Eq. (19)
Average atomic mass		28.0855 amu	Ref. [13]
Mass per atom	M	$4.7 \times 10^{-26} \text{ (kg)}$	Calculated using Ref. [13]
Strength of the mass-difference scattering	Γ	2.014×10^{-4}	
Silicon isotopes		92.2% ^{28}Si 4.7% ^{29}Si 3.1% ^{30}Si	Ref. [13]
Weight factor	η	0.55	Ref. [20]
Deformation potential	E_n	9.5 (eV)	Ref. [5]
Effective mass	m^*	$0.26 m_e$	Ref. [25]

impurity; Γ is strength of the mass-difference scattering and is equal to

$$\Gamma = \sum_i f_i \left(1 - \frac{M_i}{\bar{M}}\right)^2,$$

where f_i is fractional concentration of the impurity atoms of mass M_i and the average atomic mass is equal to $\bar{M} = \sum_i f_i M_i$. The strength for each Si isotope is given in table 3.

2.2c Phonon-boundary scattering rate: The phonon-boundary scattering rate is independent of frequency and temperature; for longitudinal and transverse modes it is given as follows [18]:

$$\left[\tau_b^{L(T)}(\omega)\right]^{-1} = \frac{v_{L(T)}}{L_{\text{eff}}}, \quad (12)$$

where L_{eff} is the effective diameter of the sample. The value of L_{eff} will be adjusted slightly in order to fit the T^3 dependence of the thermal conductivity curve at the lowest temperatures. From the experimental data used in this work as shown in figure 1, the value of L_{eff} is found to be equal to 4 mm.

For NWs the boundary scattering can be improved as follows. For absolute temperature range ($T < 10 \text{ K}$) LTC is proportional to cubical temperature, T^3 , and linearly depends on the dimension of the sample as diffused scattering is negligible [26]. The LTC decreases with decreasing sample length. The sample length could be used to modify the equation of effective phonon MFP length, L_{eff} [27]:

$$\frac{1}{L_{\text{eff}}} = \frac{1}{L_c} + \frac{1}{L}. \quad (13)$$

Figure 1. Temperature dependence of the calculated lattice thermal conductivity (solid line), fitted to the experimental data (solid circle) taken from Morelli *et al* [17], for bulk pure single crystal of Si.

In addition, assume that a fraction of phonons is scattered by surface of the sample. The relaxation rate of boundary scattering for longitudinal and transverse modes is given by [27] the relation

$$\left[\tau_B^{L(T)}\right]^{-1} = v_{L(T)} \left(\frac{1}{L_c} \frac{(1 - \varepsilon)}{(1 + \varepsilon)} + \frac{1}{L} \right), \quad (14)$$

where $1/L_{\text{eff}}$ is the specularity parameter, which depends on rate of surface roughness, ε , and the frequency of phonon. Surface roughness takes a value in the range $0 \leq \varepsilon \leq 1$, where $\varepsilon = 1$ and $\varepsilon = 0$ represent a completely specular and completely diffuse surface scattering, respectively. In the present work, for each 22, 37, 56 and 115 nm Si NW the value of ε is adjustable to fit the theoretical LTC with experimental data, but for 50, 98 and 115 nm a similar procedure yields zero value.

2.2d Phonon–dislocation scattering rate: Phonon scattering because of dislocation includes two mechanisms: the first one is short range or phonons on the core of the dislocation lines, and the second one is long range or scattering of phonons by the elastic strain field of dislocation lines interaction [8]:

$$\left[\tau_{DC}^{L(T)}(x)\right]^{-1} = \eta N_D \frac{V_o^{4/3}}{v_{L(T)}^2} \left(\frac{k_B T}{\hbar}\right)^3 x^3, \quad (15)$$

where η is a weight factor that is determined by the mutual orientation of dislocation line and temperature gradient direction, and its value is found by integration to be 0.55 [24]. N_D is the density of the dislocation lines of all types, which is given for all diameters in table 1.

2.2e Phonon–electron scattering rate: Phonon scattering rate on account of free electrons for longitudinal and transverse modes is given by [5] the relation

$$\left[\tau_{ph-e}^{L(T)}(x)\right]^{-1} = \frac{n_e E^2 x}{\rho v_{L(T)}^2 \hbar} \sqrt{\frac{\pi m^* v_{L(T)}^2}{2 k_B T}} \times \exp\left(-\frac{m^* v_{L(T)}^2}{2 k_B T}\right), \quad (16)$$

where E is the deformation potential, m^* is the effective mass of electron, n_e is the concentration density of conduction electrons and ρ is the mass density. The values of these parameters are given in tables 1–3.

3. LTC of NWs

In order to calculate LTC for quasi-one-dimensional nanostructure, the modification formula of bulk solids is needed. Size dependence is one feature that is used in this modification. Furthermore, nonequilibrium phonon distributions causing boundary scattering and acoustic phonon confinement are significant effects during this modification [5]. Phonon group velocity and phonon dispersion are two effects that regulate phonon confinement. One reason that causes phonon group velocity to quantitatively decrease with respect to its bulk counterpart is the quantization of phonon branches due to the boundary conditions at the surface in nanostructures [4,5,16]. The phonon confinement can give rise to significant decrease of LTC in nanostructures, which is demonstrated by Zou and Balandin [5]. A theoretical model that includes these effects shows agreement with experimental data [6]. Omar and Taha [13], by considering the size dependence parameter, could successfully fit theory to experimental data [6] of LTC in four Si NWs. what is more, we have used some calculation methods from Refs. [13,23] in the present work.

LTC for Si NWs has been calculated by Mingo [9] without using adjustable parameters. In his calculation the structure

of Si NWs is the same as that of the bulk crystal. In the present work, based on the results reported in Refs. [13,20,28], surface roughness, ε , Gruneisen parameter, γ , lattice dislocation density, N_D , impurity density, N_{imp} , and concentration of conduction electrons, n_e , are used as adjustable parameters. Therefore, mean bond length, d_{mean} , lattice parameter, melting temperature, T_m , vibrational entropy, S_{vib} , enthalpy of melting, H_m , lattice parameter, α , unit cell volume, V , longitudinal and transverse Debye temperature, $\theta_D^{L(T)}$, and longitudinal and transverse group velocity, $v_{T(L)}$, are calculated using equations of Ref. [23]. All these variables mentioned are size dependent.

3.1 Mean bond length

For bulk crystals usually the mean bond length, $d_{mean}(\infty)$, is constant. When the crystal size decreases to the scope of nanoscale, its value inversely depends on the size, $d_{mean}(r)$. When the value of r approaches $3h$ the mean bond length gets a critical value, $d_{mean}(r_c)$, at which the solid melts at absolute zero temperature. Thus, the change of mean bond length is as follows [29]:

$$\Delta d_{mean}(r) = \Delta d_{mean}(r_c) \left[\exp \left[\frac{-2(S_m(\infty) - R)}{3R \left(\frac{r}{r_c} - 1 \right)} \right] \right]^{1/2}, \quad (17)$$

where R is the ideal gas constant. Therefore, $\Delta d_{mean}(r_c)$ can be found when $r \rightarrow 3h$; the magnitude of h is obtaining from the following equation:

$$h = 1.429 d_{mean}(\infty). \quad (18)$$

In Eq. (17), the value of $S_m(\infty)$, which represents bulk vibrational entropy, is equal to

$$S_m(\infty) = H_m(\infty) / T_m, \quad (19)$$

where $H_m(\infty)$ is the enthalpy of melting, and can be found from the following equation:

$$H_m(\infty) = -10^{-5} T_m^2(\infty) + 0.059 T_m(\infty) - 21.33. \quad (20)$$

The size-dependent mean bond length is given by [29]

$$d_{mean}(r) = h - \Delta d_{mean}(r). \quad (21)$$

Additionally, for the bulk crystal, Eq. (21) becomes

$$d_{mean}(\infty) = h - \Delta d_{mean}(r_c). \quad (22)$$

3.2 Lattice parameter, unit cell volume and density

The result of Eqs (17) and (18) can be used in Eq. (21), to obtain the value of mean bond length for any particular NW size. Consequently, one can calculate each lattice parameter more simply as follows [22]:

$$\alpha(r) = \frac{4}{\sqrt{3}} d_{\text{mean}}(r) \quad (23)$$

and unit cell volume [28]

$$V(r) = \left[\frac{\alpha(r)}{2} \right]^3. \quad (24)$$

Lastly, the mass density is the ratio of mass over volume:

$$\rho(r) = \frac{M}{V(r)}. \quad (25)$$

3.3 Melting temperature

Using the result of Eqs (17–24), size-dependent melting temperature for semiconductors is obtained as follows [29]:

$$\frac{T_m(r)}{T_m(\infty)} = \left(\frac{V(r)}{V(\infty)} \right)^{2/3} \exp \left(- \frac{2(S_m(\infty) - R)}{3R \left(\frac{r}{r_c} - 1 \right)} \right). \quad (26)$$

Hence the parameters $S_m(\infty)$, or bulk total melting entropy, for Si can be calculated from the best fitting curve equation [29]

$$S_m(\infty) = (-10^{-5} T_m^2(\infty) + 0.059 T_m(\infty) - 21.33) / T_m(\infty). \quad (27)$$

3.4 Debye temperature and lattice group velocity

There is a relationship between Debye temperature and melting point, from Lindmann's formula, which for NWs can be written as [30,31]

$$\left(\frac{\theta_D^n}{\theta_D^B} \right)^2 = \frac{T_m^n}{T_m^B}. \quad (28)$$

What is more, lattice group velocity, using the Post [32] assumption of an isotropic system, can be expressed as

$$\frac{v^n}{v^B} = \frac{\theta_D^n}{\theta_D^B}. \quad (29)$$

Basic parameters for Si are given in table 3. The result of calculation using Eqs (17–29) is presented in table 2.

4. Analysis of results

4.1 LTC in Si bulk

For bulk Si, to calculate LTC, results of Eqs (9–16) are substituted in Eqs (2–8), which is shown in figure 1, where filled circles are experimental data from [17], and solid line is the present work. The theoretical line fits well in all regions with calculated and experimental data, except around 25 K in the 'high'-temperature region.

For calculating LTC of bulk Si, the effects taken into account are three-phonon Umklapp scattering, τ_U , isotopes and impurity, τ_M , boundary scattering τ_B and normal three-phonon scattering, τ_N [13]. Furthermore, in the present work, phonon–dislocation scattering, Eq. (15), and phonon–electron scattering, Eq. (16), are considered. The effects of both electron concentration and dislocation density in bulk Si are discussed in sections 4.4 and 4.5, respectively. Calculations show that the phonon–electron scattering has significant effect on LTC in bulk Si for value more than 10^{16} m^{-3} . Therefore, phonon–dislocation densities more than 10^{12} m^{-2} cause decrease of LTC.

4.2 LTC of Si NWs

Using Eqs (2–29), the temperature dependence of LTC of Si NWs is calculated using parameters of bulk Si given in table 3. The values of mean bond length, lattice parameter, unit cell volume, mass density, group velocities and Debye temperatures are calculated using Eqs (17–29), and the result is presented in table 2.

The diameters chosen for comparison are 115, 56, 37 and 22 nm with roughness ratio $0 \leq \varepsilon \leq 1$, presented in table 1. These particular values are correlated with experimental data [6], which are shown in figure 2.

For smooth NWs, the diameters 115, 98 and 50 nm are extracted from experimental data reported from [7], and correlated after doing all calculations performed using equations given in sections 3.1, 3.2, 3.3 and 3.4. The results are presented in table 2.

The effects of existing conduction electrons and dislocation density in calculating LTC for Si NWs start from 10^{22} m^{-3} and 10^{14} m^{-2} , respectively, as mentioned in sections 4.4 and 4.5. Furthermore, the values of other adjustable parameters are found in table 1.

Increasing relaxation rates τ_B , τ_M and τ_U decrease LTC in the range of low, middle and high temperatures, respectively.

4.3 Impurity density and surface roughness

With decreasing phonon group velocity, the scattering rate due to impurity concentration increases. It is found that rough Si NWs with diameter 115, 56 and 37 nm have approximately the same impurity density, but the 22 nm diameter sample has

Figure 2. Temperature dependence of calculated LTC for rough Si NWs with diameter (a) 115, 56, 37 and 22 nm, where k_{115T} , k_{56T} , k_{37T} , k_{22T} represent theoretical calculation of 115, 56, 37 and 22 nm and k_{115E} , k_{56E} , k_{37E} , k_{22E} represent 115, 56, 37 and 22 nm, experimental data from Ref. [6]. (b) LTC for smooth Si NWs ($\varepsilon = 0$) with diameter 115, 98 and 50 nm. The effect of boundary scattering, modified size-dependent parameters and phonon velocities has been taken into account. Symbols k_{115sE} , k_{98sE} , k_{50sE} represent 115, 98 and 50 nm, for experimental data from Ref. [7].

a greater value. Apart from this, the value of impurity for Si NW with smooth surface is larger than that of the rough Si NW with the same diameter, and with the diameter decreasing in the order 115, 98 and 50 nm, larger value of N_{imp} has to be assumed (figure 3a).

Asen-Palmer *et al* [18] showed that surface roughness has a significant effect on controlling LTC of NWs in low-temperature region, with respect to the bulk [33]. In addition, Ziman [34] illustrates the power of varying rate of surface polishing on LTC as a function of temperature. Variation of surface roughness parameter as a function of diameter of Si is shown in figure 3b.

Figure 3. (a) Impurity densities obtained in this work for rough Si NWs with diameter 22, 37, 56 and 115 nm (filled squares), and for smooth Si NWs 50, 98 and 115 nm (filled circles). (b) Surface roughness for Si NWs with diameter 22, 37, 56 and 115 nm. The value of roughness increases with increasing diameter.

4.4 Concentration of conduction electron

Concentration of conduction electron, n_e , has no effect for values less than 10^{16} m^{-3} , in bulk Si; incidentally, for NWs with decreasing diameters and value of roughness, more n_e is needed in relation to bulk to display its quantitative effect on LTC. From figure 4 it can be concluded that n_e depends on surface roughness and size-dependent parameter. Although, there are possibilities of electron-phonons scattering, it has been stated that for carrier concentrations less than 10^{25} m^{-3} there will be no thermal conductivity due to electrons [35].

4.5 Dislocation density

The effect of dislocation density, N_D , for all rough and smooth Si NWs is shown in figure 5, which exhibits the maximum amount of N_D for each diameter. For bulk Si, as recorded in table 1, it can be obviously seen that the effect of dislocation density starts from the value 10^{12} m^{-2} . LTC for N_D more than this value decreases rapidly and for values less than this value it is not affected.

Figure 4. Concentration of conduction electrons vs. diameter for rough Si NWs with diameters 22, 37, 56 and 115 nm, and smooth Si NWs with diameters 50, 98 and 115 nm.

Figure 5. Dislocation density vs. diameter for rough Si NWs with diameters 22, 37, 56 and 115 nm, and smooth Si NWs with diameters 50, 98 and 115 nm.

The effect of N_D for the Si NWs starts at 10^{14} m^{-2} for 115 nm and $2 \times 10^{15} \text{ m}^{-2}$ for 22 nm. It is shown that this is also another size-dependent parameter, which can be formulized in the future works. Likewise, with decreasing diameter of smooth Si NWs, more value of N_D is needed in order to decrease the LTC.

5. Conclusions

In the temperature range of 3–300 K, numerical calculations for rough and smooth Si NWs with diameters (22, 37, 56 and 115) and (50, 98 and 115 nm) have been performed, respectively. The significant decrease of LTC is due to boundary scattering, which increases thermal resistivity of Si NWs. The decrease in wires diameter causes increase of group velocity, Debye temperature, melting temperature and mass density. However, mean bond path, lattice parameter and unit cell volume decrease in proportion to the reduction of the diameter of Si NWs.

Apart from these, phonon–electron scattering can affect LTC in low-temperature region when the value of electron concentration, n_e , is more than 10^{16} for bulk and 10^{22} for NWs. In addition, dislocation–phonon scattering affects the maximum value of LTC peak and causes a significant reduction. The value of N_D for Si NWs and bulk has been found—it is 10^{12} for bulk and 10^{14} for NWs. Hence, any number less than these values does not affect the curves.

Theoretical values of impurity, dislocation, electron concentration and longitudinal and transverse Gruneisen parameters for Si bulk and NWs correlate with experimental results. Furthermore, Casimir length and sample length were found from literature; surface roughness parameter for 22, 37, 56 and 115 nm diameter NWs was obtained and for smoothness surfaces of 50, 98 and 115 nm diameter NWs, it is assumed to be zero.

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