B. J. Abdullah

Department of Physics, College of Science, University of Salahaddin,
Arbil, Iraq Kurdistan, Iraq
E-mail: Botan_nano@yahoo.com

Effect of Size on Lattice Thermal Conductivity in Si and Ge Nanowires from 2K to room temperatures

Lattice thermal conductivity in silicon and germanium nanowires of diameters 22, 37, 56 and 115nm were theoretical investigated in the temperature range between 2K to 300K. Size dependence of melting point, Debye temperature and group velocity of silicon and germanium nanowires determined and it drops with decreasing their size. The size effects on the lattice thermal conductivity is calculated using the Debye-Callaway model modified to include both longitudinal and transverse phonon modes explicitly with the strong effect of scattering of phonons by sample boundaries, mass-differnce and other phonons via both normal and umklapp process and also the modification of Gruneisen parameter, lattice dislocation and surface roughness is considered. The results show that lattice thermal conductivity of Si and Ge nanowires can be significantly smaller than the bulk with reduction of nanowire diameters, the approach yields good agreement with experimental results for Si nanowires, for Ge nanowires of the same diameters are given and exhibit a lower lattice thermal conductivity than silicon, enabling future experimental verification.

1. Introduction

In the past two decades, a lot of attention has been paid to the low-dimensional materials because of their demand for miniaturization of electronic devices and the desired thermal as well as electric properties for thermoelectric applications [1, 2]. It was realized that low-dimensional materials can possibly result in a higher power factor because of the size-quantization effects and electron energy filtering [3] and in lower thermal conductivity as the lattice wave are confined when the characteristic length scale of the materials is smaller than or comparable to the phonon mean free path. Among all the differences in the thermoelectric properties between nanowires and bulk materials are expected to be most substantial due to large surface-to-volume ratio of nanowires [4, 5]. Semiconducting silicon and germanium nanowires have raised interest as promising building blocks for nanoscale electronic devices and more recently, as efficient thermoelectric materials [6].

Determining the thermal conductivity of semiconducting nanowires plays a crucial role in the development of a new generation of thermoelectric materials [7]. Historically, lattice thermal conductivity in crystalline materials has been derived by: Callaway[8] developed based on the single mode relaxation time model that can successfully predict the low temperature thermal conductivity of germanium, this approach uses the Debye approximation, which assumes that there is no phonon dispersion and that the longitudinal and transverse polarizations behave identically and he pointed out that because normal processes cannot by themselves lead to finite lattice

thermal conductivity, it is not legitimate to add reciprocal relaxation times for normal processes. And later Holland[9] extended the work of Callaway by separating the contributions of longitudinal acoustic and transverse acoustic phonon, including some phonon dispersion and using different forms of the relaxation times, better high temperature agreement was found for germanium than with Callaway model. Callaway's [8] and Holland's [9] model have been used by Asen-Palmer et al. [10] for the thermal conductivity analysis to estimate the effect of isotopes and normal processes of the phonon scattering, which they have modified the callaway model to get satisfactory fits to their experimental data on germanium. In their approach, they treat transverse and longitudinal modes separately and presented the most widely used formulation for bulk lattice thermal conductivity k(T) for various semiconductors.

Lattice Thermal conductivity for intrinsic crystal Si nanowires of different diameters 22, 37, 56 and 115nm have been measured by Li et al. [11]. The results show that for all four-diameter wires the lattice thermal conductivity are much lower than bulk value and at their smallest wire diameter of 22nm, a linear lattice thermal conductivity appears over the whole temperature range. Most of researchers were calculated lattice thermal conductivity for Si nanowires of different diameters of 37, 56 and 115nm, they were successful for some of these diameters compared to the experimental data but none of them succeeded to obtain an accurate value for the 22nm diameter.

The purpose of this paper is to calculate the lattice thermal conductivity using an approach similar to that of Asen-Palmer et al.[10] with size effects of melting point, Debye temperature, group velocity and the effect of modification on Gruneisen parameter, lattice dislocation and surface roughness on the lattice thermal conductivity in Si and Ge nanowires, good agreement with experimental results is obtained for Si nanowires. On the other hand, followed the same method as for Si nanowires, to obtain the lattice thermal conductivity sets of Ge nanowires by recalculation and using the same theoretical dependencies, for which no experimental data is available to date, which await experimental verification.

2. Theoretical Model

2.1 Lattice thermal conductivity. Recently an extension of the Callaway model was provided by Asen-Palmer et al.[10], who successfully modeled the lattice thermal conductivity by not only using the Callaway formalism but also by considering the explicit mode dependence of the lattice thermal conductivity and summing over one longitudinal (κ_L) and two degenerate transverse (κ_T) phonon branches:

$$\kappa = \kappa_L + 2\kappa_T . \tag{1}$$

Based on the Callaway's[8] model, κ_L can be written as

$$\kappa_L = \kappa_{L1} + \kappa_{L2}, \tag{2}$$

where

$$\kappa_{L1} = \frac{1}{3} C_L \int_0^{\theta_L/T} \frac{\tau_C^L(x) x^4 e^x}{(e^x - 1)^2} dx, \tag{3}$$

$$\kappa_{L2} = \frac{1}{3} C_L \frac{\left[\int_0^{\theta_L/T} \frac{\tau_C^L(x) x^4 e^x}{\tau_N^L(x)(e^x-1)^2} dx \right]^2}{\int_0^{\theta_L/T} \frac{\tau_C^L(x) x^4 e^x}{\tau_N^L(x)\tau_R^L(x)(e^x-1)^2} dx}. \tag{4}$$

As for transverse branch

$$\kappa_T = \kappa_{T1} + \kappa_{T2} \tag{5}$$

where

$$\kappa_{T1} = \frac{1}{3} C_T \int_0^{\theta_T/T} \frac{\tau_C^T(x) x^4 e^x}{(e^x-1)^2} dx, \tag{6}$$

$$\kappa_{T2} = \frac{1}{3} C_T \frac{\left[\int_0^{\theta_T/T} \frac{\tau_C^T(x) x^4 e^x}{\tau_N^T(x)(e^x-1)^2} dx \right]^2}{\int_0^{\theta_T/T} \frac{\tau_C^T(x) x^4 e^x}{\tau_N^T(x)\tau_R^T(x)(e^x-1)^2} dx}. \tag{7}$$

In these expressions, $(\tau_N)^{-1}$ is the scattering rate for normal phonon processes, $(\tau_R)^{-1}$ is the sum of all resistive scattering processes such as isotope, three-phonon Umklapp and boundary, and $(\tau_C)^{-1}$ is the combined relaxation rate that can be written as

$$(\tau_C)^{-1} = (\tau_N)^{-1} + (\tau_R)^{-1}, \tag{8}$$

where subscript T and L denote transverse and longitudinal phonons, T is absolute temperature, θ_L and θ_T are Debye temperatures of transverse and longitudinal branches respectively, x is a dimensionless parameter that can be written as

$$x = \frac{\hbar\omega}{k_B T} \tag{9}$$

where ω is phonon frequency, $\hbar$ is reduced Planck constant and k_B is the Boltzmann constant.

And

$$C_{L(T)} = \frac{k_B^4}{2\pi^2 \hbar^3 v_{L(T)}}. \tag{10}$$

Here $v_{L(T)}$ are the longitudinal (transverse) acoustic phonon velocities, respectively.

2.2 Phonon relaxation rates. In this model, the acoustic phonon relaxation is considered in resistive processes, such as three-phonon Umklapp scattering, mass-difference scattering, boundary scattering and normal three-phonon scattering. The relaxation times are τ_U, τ_M, τ_B and τ_N respectively. The effective relaxation rate can be obtained by the Matthiessen rule for each phonon mode

$$(\tau_C^L)^{-1} = (\tau_U^L)^{-1} + (\tau_M^L)^{-1} + (\tau_B^L)^{-1} + (\tau_N^L)^{-1} \tag{11}$$

and

$$(\tau_C^T)^{-1} = (\tau_U^T)^{-1} + (\tau_M^T)^{-1} + (\tau_B^T)^{-1} + (\tau_N^T)^{-1}. \tag{12}$$

The relaxation rate for phonon-phonon Umklapp scattering was given by Slack and Galginaitis [12] as

$$\tau_U^{-1}(\omega) = B_U \omega^2 T e^{(-\theta_D/3T)} \tag{13}$$

with

$$B_U = \frac{\hbar\gamma^2}{Mv^2\theta_D}, \tag{14}$$

where γ is the Gruneisen anharmonicity parameter and M is the average atomic mass in the system. The phonon-phonon relaxation rates in the case of longitudinal and transverse phonons are expressed in terms of the dimensionless parameter x as

$$(\tau_U^L(x))^{-1} = B_U^L (\frac{k_B}{\hbar})^2 T^3 e^{(-\theta_L/3T)} \tag{15}$$

with

$$B_U^L = \frac{\hbar {\gamma_L}^2}{M {v_L}^2 \theta_L} \tag{16}$$

and

$$(\tau_U^T(x))^{-1} = B_U^T (\frac{k_B}{\hbar})^2 T^3 e^{(-\theta_T/3T)} \tag{17}$$

with

$$B_U^T = \frac{\hbar {\gamma_T}^2}{M {v_T}^2 \theta_T}. \tag{18}$$

The Umklapp scattering rate depends on the longitudinal and transverse Debye temperatures θ_L and θ_T, acoustic phonon velocities v_L and v_T, and Gruneisen parameters γ_L and γ_L, thus will be different for different modes and it is assumed that heat is carried only by acoustic phonons, where bulk values γ^L and γ^T of silicon and germanium equal to 1.1 and 0.6[10] respectively.

Mass-difference scattering is the scattering of phonon due to differences in mass. The mass-difference scattering rate is given by Klemens[13]

$$\tau_M^{-1}(\omega) = \frac{V_o \Gamma \omega^4}{4\pi v^3} + \frac{3V_o^2 S^2}{\hbar v^3} N_{imp} \tag{19}$$

where V_0 is the volume per atom, S is the scattering factor which usually has a value close to unity, N_{imp} is the impurity concentration. However impurity concentration up to 10^{17}cm^{-3} has no effect on lattice thermal conductivity in bulk crystal. Γ is the measure of the strength of the mass-difference scattering defined as

$$\Gamma = \sum_i f_i (1 - \frac{M_i}{\bar{M}}) \tag{20}$$

Here f_i is the fractional concentration of the impurity atoms of mass M_i, and

$$\bar{M} = \sum_i M_i f_i, \tag{21}$$

where $\bar{M}$ is the average atomic mass. Naturally occurring silicon consists of three main isotopes having their atomic masses of 27.976929, 28.976496 and 29.973763, while naturally occurring germanium of five isotopes have 69.9243, 71.9217,

72.9234, 73.9219 and 75.9214. Mass-difference relaxation rates in the case of longitudinal and transverse phonons are expressed in terms of the dimensionless parameter x as

$$(\tau_M^L(x))^{-1} = \frac{V_o k_B^4}{4\pi\hbar^4 v_L^3} x^4 T^4 + \frac{3V_o^2 S^2}{\hbar v_L^3} N_{imp} \tag{22}$$

and

$$(\tau_M^T(x))^{-1} = \frac{V_o k_B^4}{4\pi\hbar^4 v_T^3} x^4 T^4 + \frac{3V_o^2 S^2}{\hbar v_T^3} N_{imp}. \tag{23}$$

The phonon-boundary scattering rate is assumed independent of temperature and frequency and can be written as[10,13]

$$\tau_B^{-1} = \frac{v}{D}, \tag{24}$$

where D is the diameter of nanowires. Zou and Balandin[14] includes effect resulting from specular reflection of phonon at the surface, they introduced the parameter p, which characterizes the interface roughness and its effect on the boundary scattering. The value of p represents the probability that the phonon is undergoing a specular scattering event at the interface. The value of $(1-p)$ represents the probability that the phonon is undergoing a diffuse scattering event. Then the expression for the boundary scattering rate via introduction of parameter p, is taken as [14]

$$\tau_B^{-1} = \frac{v}{D}(1-p). \tag{25}$$

The boundary scattering rates in the case of longitudinal and transverse phonons which interest in this paper are expressed in terms of the specularity parameter p as

$$(\tau_B^L)^{-1} = \frac{v_L}{D}(1-p) \tag{26}$$

and

$$(\tau_B^T)^{-1} = \frac{v_T}{D}(1-p). \tag{27}$$

The normal phonon scattering do not contribute directly to the thermal resistance but are crucial in spreading out the influence of the other resistive processes to the entire phonon spectrum. For phonon-phonon normal scattering the relaxation rate [13, 15]

$$\tau_N^{-1}(\omega) = B_N \omega^a T^b \tag{28}$$

is the general form suggested by best fits to experimental thermal conductivity data; the scattering rate coefficient B_N is a constant independent of ω and T with (a, b) = (1, 4) and (2, 3) were used for group IV and III-V semiconductors for longitudinal and transverse phonon, respectively. The approach of Asen-Palmer et al. [10] are the appropriate forms for longitudinal and transverse phonons, and expresses as

$$(\tau_N^L(x))^{-1} = B_N^L (\frac{\kappa_B}{\hbar})^2 x^2 T^5 \tag{29}$$

with

$$B_N^L = \frac{\kappa_B^3 \gamma_L^2 V_o}{M\hbar^2 v_L^5} \tag{30}$$

and

$$(\tau_N^T(x))^{-1} = B_N^T(\frac{\kappa_B}{\hbar})xT^5 \tag{31}$$

with

$$B_N^T = \frac{\kappa_B^4 \gamma_T^2 V_o}{M\hbar^3 v_T^5}. \tag{32}$$

2.3 Phonon group velocities. The average phonon velocity v is proportional to the characteristic Debye temperature θ_D of a crystal[16]

$$\theta_D \alpha \frac{2h}{\pi k_B}\left(\frac{3N_A}{4\pi V}\right)^{1/3} v \tag{33}$$

with the Plank constant *h*, the Avogadro constant N_A and the molar volume V. The system considered is assumed to be isotropic. By using the subscript B and n which means the corresponding bulk and nanowires crystal respectively, the size dependence of the phonon velocity is equal to that of the Debye temperature

$$\frac{v^n}{v^B} = \frac{\theta_D^n}{\theta_D^B}. \tag{34}$$

Lindemann's [17] proposed the relation between the melting point and the Debye temperature of crystals, starting that a crystal will melt when the root mean square displacement of atoms in the crystal exceeds a certain fraction of the inter-atomic distance for small particles. Combining with the Einstein specific heat theory, the square of the characteristic temperature is proportional to the melting point T_m of crystals, and the modern from of this relation for the Debye temperature is

$$\theta_D = const \cdot \left(\frac{T_m}{MV^{2/3}}\right)^{1/2} \tag{35}$$

with the molecular mass M, According to the same relation for nanowires[16]

$$\frac{\theta_D^n}{\theta_D^B} = \frac{T_m^n}{T_m^B} \tag{36}$$

where T_m^n, T_m^B, θ_D^n and θ_D^B are the melting points and Debye temperatures of the nanowires and the corresponding bulk crystals, respectively. The size dependent melting point is calculated from the relation [18]

$$\frac{T_m^n}{T_m^B} = \exp\left(-\frac{2(S_m - R)}{3R(r_n/r_o - 1)}\right), \tag{37}$$

where S_m is the bulk over all melting entropy and R is the molar gas constant and equal to 8.314 $J.K^{-1}.mol^{-1}$, r_n is the radius of nanowires and r_o is the critical radius of which all atoms of the particle are located on its surface. For low dimension crystals,

Table 1. *Calculated size dependency (ν, θ_D and T_m) for silicon by using equations (34), (36) and (37).*

Diameter D (nm)	Melting point T_m (K)	Debye temperature θ_D (K)		Group velocity ν x10^3 (m/sec)	
		θ_D^L	θ_D^T	ν^L	ν^T
Bulk	1690	586	240	8.476	5.850
115	1655.500	579.986	237.537	8.390	5.790
56	1619.047	573.566	234.907	8.300	5.729
37	1582.460	567.050	232.238	8.202	5.660
22	1508.666	553.670	226.758	8.008	5.527

it is clear that r_o in equation (37) should be dependent on the structure dimension d: where $d = 0$ for nanocrystals, 1 for nanowires and 2 for the thin films. The relation between d and r_o is given by

$$r_o = (3-d)a_o, \tag{38}$$

where a_o is the atomic diameter.

3. Result of simulation and discussion.

Values T_m^n, T_m^B, θ_D^n, θ_D^B, ν^n and ν^B are calculated through equations (34), (36) and (37) and displayed in Tables (1) for silicon and (2) for germanium and they are used in present calculation, the result indicate that it drops with decreasing their diameter. The material parameters characteristic of silicon and germanium used in the calculations for the longitudinal and transverse acoustic wave are $v_L = \sqrt{C_{11}/\rho}$ and $v_T = \sqrt{C_{44}/\rho}$, where C_{11}, C_{44} are elastic constants for silicon and germanium equal to $16.74\cdot10^{11}$, $7.96\cdot10^{11}$dyne/cm^2 and $12.90\cdot10^{11}$, $6.70\cdot10^{11}$ dyne/cm^2 respectively and ρ is the material density for silicon and germanium is 2.33 and 5.36g/cm^3 respectively.

Table. 2. *Calculated size dependency (ν, θ_D and T_m) for germanium by using equations (34), (36) and (37).*

Diameter D (nm)	Melting point T_m (K)	Debye temperature θ_D (K)		Group velocity ν x10^3 (m/sec)	
		θ_D^L	θ_D^T	ν^L	ν^T
Bulk	1210	333	150	4.750	3.535
115	1184.271	329.440	148.396	4.700	3.497
56	1157.082	325.636	146.683	4.645	3.456
37	1129.800	321.775	144.943	4.590	3.415
22	1065.462	312.478	140.756	4.457	3.317

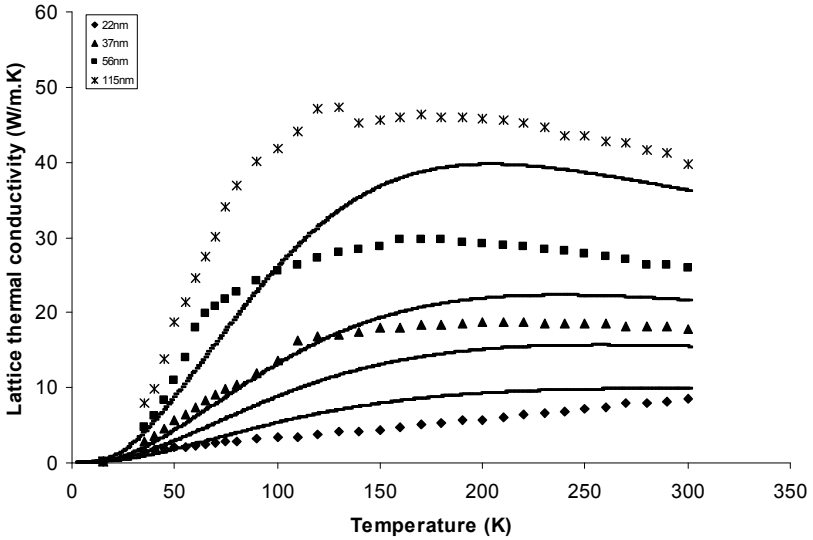

Fig. 1. *Calculated lattice thermal conductivity versus temperature from 2 to 300 K for silicon nanowires of diameters 22, 37, 56 and 115 nm by using the effect of all scattering and calculated phonon group velocity, Debye temperature and melting point in comparison with that of the experimental data[11].*

The critical radius r_o is calculated from equation (38) for silicon and germanium is 0.674 and 0.0702nm respectively and the atomic diameter a_o for silicon and germanium is estimated from the formula $a^3 = 4\pi a_o^{\,3}/3$ is 0.337 and 0.351nm, respectively.

In this work the scattering processes of Umklapp, mass-difference and boundary contributes to lattice thermal conductivity were considered. The effect of temperature dependent lattice thermal conductivity k for diameters 22, 37, 56 and 115 nm numerically calculated using MathCAD Software to solve equation (1) are presented in Fig.(1) and Fig.(2) for silicon and germanium respectively, the result shows the varia-

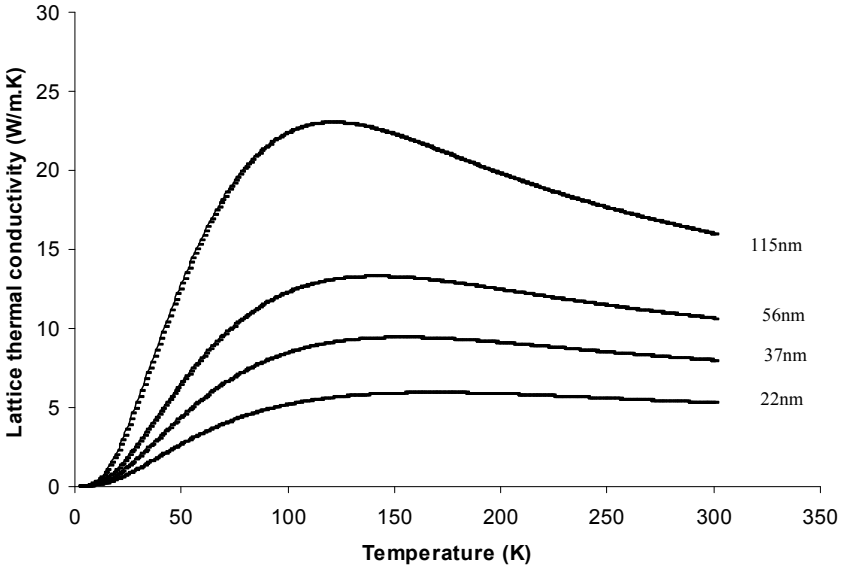

Fig.2. *Calculated lattice thermal conductivity versus temperature from 2 to 300 K for germanium nanowires of diameters 22, 37, 56 and 115nm by using the effect of all scattering and calculated phonon group velocity, Debye temperature and melting point.*

tions of the lattice thermal conductivity with different diameters and values of lattice thermal conductivity for intrinsic single crystal silicon will be compared with that of the reported experimental data [11].

The other parameters used in the numerical solution are the form factor for the mass-difference of three silicon isotopes was found to be 0.922, 0.047 and 0.031 and for five germanium isotopes equal to 0.205, 0.274, 0.078, 0.365 and 0.078, the measure of the strength of the mass-difference scattering Γ of silicon and germanium is calculated from equation (20) which is equal to $2.012\cdot10^{-4}$ and $5.874\cdot10^{-4}$ respectively, the average atomic mass of silicon and germanium is calculated from equation (21) is 28.0858 and 72.6324 atomic mass unit respectively and the volume per atom V_o of silicon and germanium having their lattice constant a of 5.66 and 5.43 Å is estimated from the formula $V_o = a^3/8$ is $2.0012\cdot10^{-29}$ and $2.2665\cdot10^{-29}$ m^3 respectively.

Due to other size dependence parameters some other mechanism comes in and plays an important role for the phonon transport such as N_{imp}, P and γ where their explanations are given in the following section:

3.1 Modification due to Lattice Dislocations, Surface roughness and Gruneisen anharmonicity parameters on lattice thermal conductivity. When a bulk crystal reduces to a nanowire size, the geometrical disturbance is expected to occur and the periodicity of the lattice from wire cross-section center increases in a systematic form from the minimum inter-atomic bonding which is mostly for the bulk to that of the maximum bonding length at the surface[19]. Lattice arrangement of successive circular layers at the wire cross-section will be deformed with regard of their lattice periodicity by transferring from the expected surface plane to another at their truncate. However, truncate makes an intersection angle between the two planes where it increases as the wire diameter decreases[20].

Both assumed suggestions causes increase in the degree of dislocation with the decrease of diameter. According to this approach, the properties related to the surface will remain constant the ones belong to the bulk change in accordance to its percentage surface to bulk ratio. The best fit values obtained for the concentration of lattice dislocation versus diameters of silicon nanowires are $1.17\cdot10^{19}$, $12.52\cdot10^{19}$,

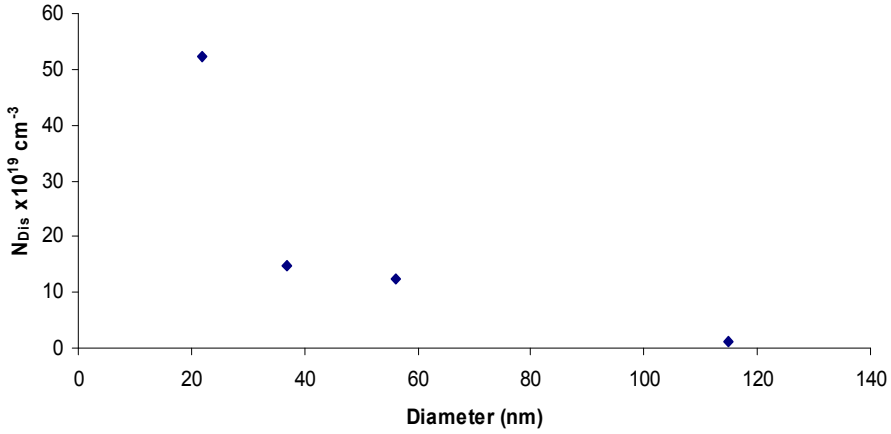

Fig.3. *The diameter dependence of lattice dislocation of silicon nanowires.*

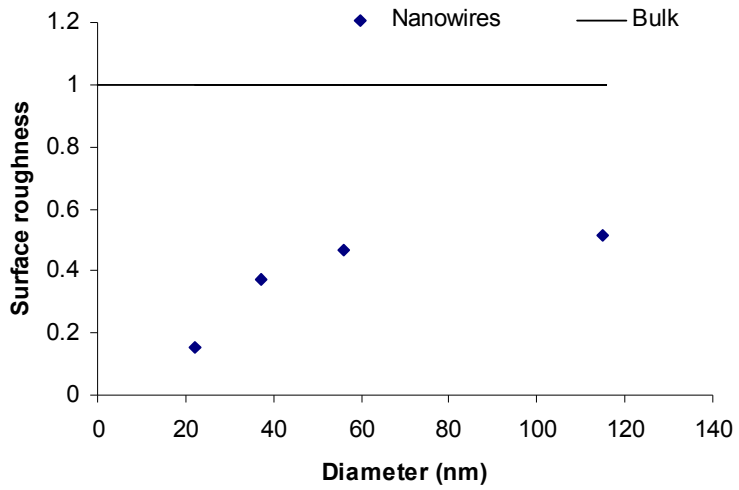

Fig. 4. *The surface roughness versus silicon nanowire diameter.*

14.83×10^{19} and $52.34 \times 10^{19} cm^{-3}$ respectively, in this case the dislocation concentration versus silicon nanowire diameter is shown in Fig.(3) and the result indicated that values of lattice dislocation increases as the diameter of silicon nanowires decreases.

The other parameter affect on lattice thermal conductivity which influence the boundary scattering is the surface roughness, the best fit values obtained for the surface roughness versus diameters of silicon nanowires ranged between $0.512 \leq p \geq 0.154$ are 0.512, 0.468, 0.374 and 0.154, the result indicated that values of p decreases as the diameter of silicon nanowires decreases as shown in Fig.(4) and this leads to higher probability of diffuse scattering.

When the size of a crystal reduces to a nanoscale range, the surface to bulk ratio begins to effect the mechanical properties of the material and the surface bonding length is much larger than that for the bonds belong to the bulk material[18], thus surface effects in these high surface to volume ratio will become important on lattice thermal conductivity, the probability of controlling lattice thermal conductivity by Gruneisen anharmonicity parameter in nanoscale size system would be possible. Such a conclusion can be used to correlate of both longitudinal and transverse Gruneisen anharmonicity parameter. The best fit values obtained for the γ^L and γ^T versus diameters of silicon nanowires are 1.248, 1.456, 1.597 and 1.802 and 0.687, 0.952, 1.143, and 1.483 respectively, the result indicated that values of γ^L and γ^T increases as the diameter of silicon nanowires decreases as shown in Fig.(5) and Fig.(6).

After modification in Gruneisen anharmonicity parameter, lattice dislocation and surface roughness, good agreement with experimental results is obtained for Si nanowires as shown in Fig.(7) and for the germanium nanowires the modified theoretical curves are obtained with the effect of modification and recalculation on the lattice thermal conductivity directly from the parameters proportionality for silicon nanowires to that of germanium by using the same theoretical dependencies as shown in Fig.(8), the result shows that as the wire diameter goes down the corresponding lattice thermal conductivity is decreases, comparison with result of silicon nanowires in Fig.(7) shows that the lattice thermal conductivity of the germanium nanowires are much lowers than of silicon of similar diameter.

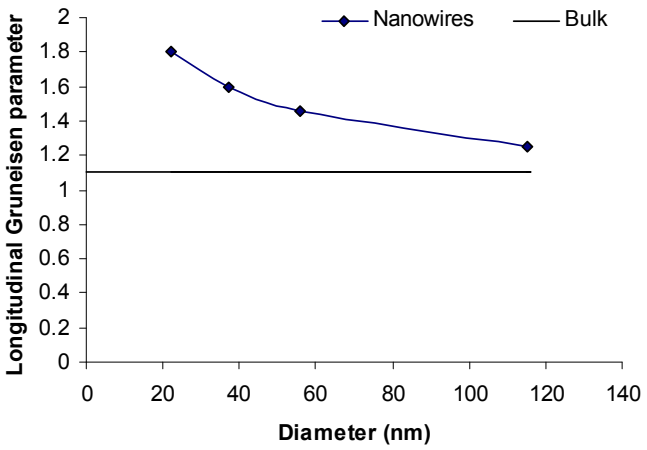

Fig.5. *The longitudinal Gruneisen parameter as a function of nanowire diameter for silicon.*

4. Conclusions

In this paper, the parameters which used in calculation nanowires material are no longer constant such as group velocity, Debye temperature and melting point but change depend on the nanowires size and the deviation of calculated lattice thermal conductivity from that of the experimental values are controlled by the modified bulk values of the surface roughness, lattice dislocation and Gruneisen anharmonicity parameters.

The lattice thermal conductivity of silicon and germanium nanowires observed to decrease as the diameter is reduced. In comparison to silicon nanowires for the same diameters, lattice thermal conductivity is about 1/2 of its value for germanium nanowires, this is due to difference in isotop, lattice dislocation, boundary and Gruneisen anharmonicity parameter where all of them increase the phonon scattering rate, hence, a reduced lattice thermal conductivity.

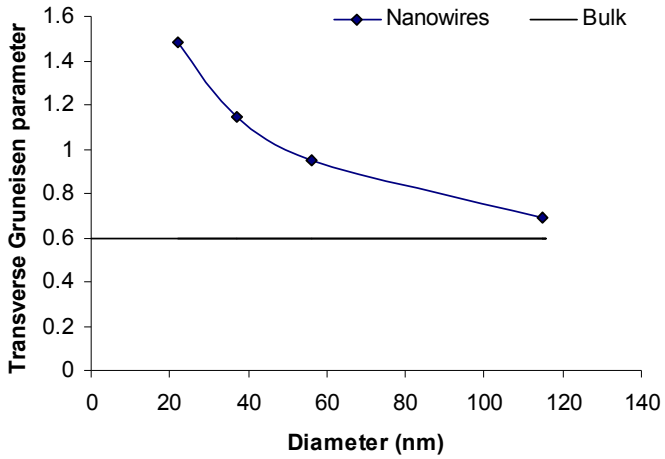

Fig.6. *The Transverse Gruneisen parameter as a function of nanowire diameter for silicon.*

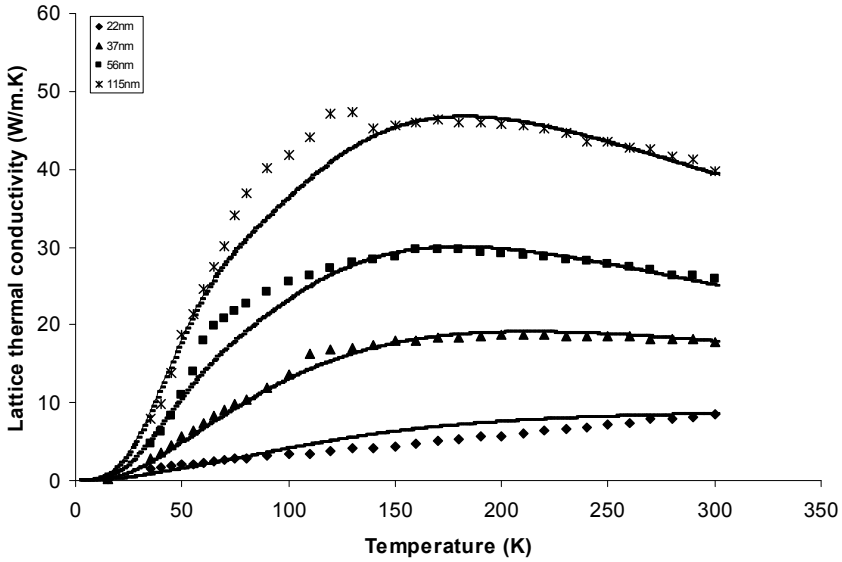

Fig.7. *Calculated lattice thermal conductivity versus temperature from 2 to 300 K for silicon nanowires of diameters 22, 37, 56 and 115nm by using the effect of all scattering and calculated phonon group velocity, Debye temperature and melting point as well as the size dependent parameters of lattice dislocation, surface roughness and Gruneisen parameter in comparison with that of the experimental data [11].*

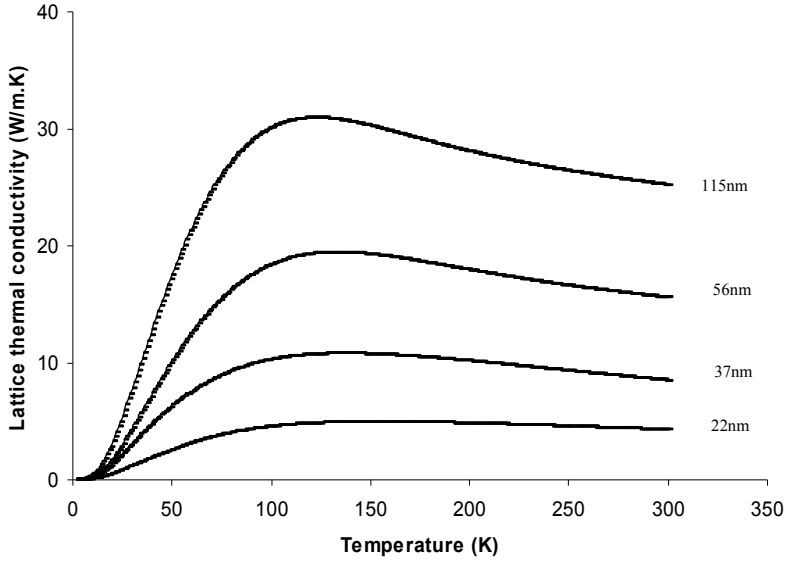

Fig.8. *Modification and recalculation lattice thermal conductivity versus temperature from 2 to 300 K for germanium nanowires of diameters 22, 37, 56 and 115nm by using the effect of all scattering and calculated phonon group velocity, Debye temperature and melting point well as the size dependent parameters of lattice dislocation, surface roughness and Gruneisen parameter.*

References

1. *D.G. Cahiila, W.K. Ford, K.E. Goodson, G.D. Mahan, A. Majumdar, H.J. Maris, R. Merlin, S.R. Philpot* Nanoscale thermal transport. J. Appl. Phys. 93 (2003) 793-818.
2. *J.P. Heremans* Low-dimensional thermoelectricity, Acta Phy. Pol. A 108 (2005) 609-634.
3. *L.D. Hicks, M.S. Dressselhaus* Thermoelectric figure of merit of a one-dimensional conductor, Phys. Rev. B 47 (1993) 16631-16634.
4. *Khitun, A. Balandin, K.L. Wang* Modification of the lattice thermal conductivity in silicon quantum wires due to spatial confinement of acoustic phonons, Superlattices Microstruc. 26 (1999) 181-193.
5. *M.J. Huang, T.M. Chang, W.Y. Chong, C.K. Liu, C.K. Yu* A new lattice thermal conductivity model of a thin film semiconductor, Int. J. Heat and Mass Transf. 50 (2007) 67-74.
6. *Bjorn Marsen, Klaus Satter* Fullerene-structured nanowires of silicon, Phys. Rev. B, 60 (1999) 11593-11600.
7. *G. Muhan, B. Sales, J. Sharp* Thermoelectric materials: New approaches to an old problem, Phys. Today, 50 (1997) 42-47.
8. *J. Callaway* Model for lattice thermal conductivity at low temperatures, Phys. Rev. 113 (1959) 1046-1051.
9. *M Holland* Analysis of lattice thermal conductivity, Phys. Rev. 132 (1963) 2461-2471.
10. *M. Asen-Palmer, K. bartkowski, E. Gmelin, M. Cardona, A.P. Zherno, A.V. Inyushkin, A. Taldenkov, V.I. Ozhogin, K.M. Iton, E.E. Haller* Thermal conductivity of germanium crystals with different isotopic compositions, Phys. Rev. B 56 (1997) 9431-9447.
11. *D. Li, Y. Yu, P. Kim, L. Shi, N. Mingo, Y. Liu, P. Yang, and A. Majumdar* Thermal conductivity of individual silicon nanowires, Appl. Phys. Lett. 83 (2003) 2934-2936.
12. *G.A. Slack, S.S. Galginaitis* Thermal conductivity and phonon scattering by magnetic impurities in CdTe, Phys. Rev. 133 (1963) 253-268.
13. *P.G. Klemens* Thermal conductivity and lattice vibration modes, Solid State Physics, Vol. 7 (1958) 1-98.
14. *Jie Zou, Alexander Balandin* Phonon heat conduction in a semiconductor nanowires, Apply. Phys. 89 (2000) 2932-2938.
15. *R. Berman* Thermal Conduction in Solids, Clarendon Press., Oxford (1976).
16. *L.H. Liang, Baowen L*, Size-dependent thermal conductivity of nanoscale semiconducting systems, Phys. Rev. B 73 (2006) 153303-153306.
17. *F.A. Lindemann* The calculation of molecular vibration frequency, Z. Phys. 11 (1910) 609-612.
18. *Z. Zhang, M. Zhao, Q. Jiang* Melting temperatures of semiconductor nanocrystals in the mesoscopic size range, Semicond. Sci. Technol, 16 (2001) L33-L35.
19. *M.S. Omer* Lattice thermal expansion for normal tetrahedral compound semiconductors, Materials Res. (2007) Bull. 42: 319-326.

20.*Lee B, Rudd R.E.* First-principles study of the young's modulus of Si (001) nanowires, Phys. Rev. (2007) B75: 041305-041308(R).

Б. Д. Абдулах

Влияние размера на теплопроводность решетки в нанопроволоках Si и Ge в диапазоне температур от 2 К до комнатной

АННОТАЦИЯ

Теоретически исследована теплопроводность пространственных решеток нанопроволок Si и Ge диаметром 22, 37, 56 и 115 нм в температурной диапазоне 2÷300 К. Определены зависимости размера нанопроволок Si и Ge от температуры плавления, температуры Дебая и групповой скорости, и установлено снижение последних с уменьшением диаметра. Влияние размера на теплопроводность пространственной решетки оценено в рамках модели Дебая - Каллавея, с учетом продольных и поперечных фононных мод с ярко выраженным эффектом рассеяния фононов на границах образца, а также исследовано влияние дислокаций решетки, шероховатости поверхности и изменение параметра Грюнайзена. Как следует из полученных результатов, теплопроводность решеток нанопроволок Si и Ge может быть значительно меньше ее значения в объеме. В рамках работы показано хорошее соответствие результатов известным экспериментальным данным для нанопроволок Si таких же диаметров. В свою очередь, меньшая теплопроводность решеток нанопроволок Ge по сравнению с Si в дальнейшем требует экспериментальной проверки.

Б.Д. Абдулах

Вплив розміру на теплопровідність решітки в нанодротиках Si та Ge в діапазоні температур від 2 К до кімнатної

АНОТАЦІЯ

Теоретично досліджено теплопровідність просторових решіток нанодротів Si і Ge діаметром 22, 37, 56 і 115 нм в температурному діапазоні 2 ÷300 К. Визначено залежності розміру нанодротів Si і Ge від температури плавлення, температури Дебая та групової швидкості, і встановлено зниження останніх із зменшенням діаметра. Вплив розміру на теплопровідність просторової решітки оцінений в рамках моделі Дебая - Каллавея, враховуючій також поздовжні і поперечні фононні моди з яскраво вираженим ефектом розсіювання фононів на межах зразка, а також досліджено вплив дислокацій решітки, шорсткості поверхні та зміни параметра Грюнайзена. Як випливає з отриманих результатів, теплопровідність решіток нанодротів Si і Ge може бути значно менше значення в об'ємі. У рамках роботи показана хороша відповідність результатів відомим експериментальним даним для нанодротів Si таких же діаметрів. У свою чергу, менша теплопровідність решіток нанодротів Ge в порівнянні з Si надалі вимагає експериментальної перевірки.