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RESEARCH PAPER

The influence of Surface Roughness on the Lattice thermal Conductivity in Silicon Nanowires

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A B S T R A C T:
A modified model is proposed to account for the effects of roughness on lattice thermal conductivity (LTC) in Si nanowires (SiNWs). Depending on the modification of the Debye-Callaway models effects of surface roughness is carried out to predict LTC in SiNWs. Through the process of fitting the calculated curve to that of the reported experimental data, phonon scattering strength from the boundary, Umklapp-normal phonon–phonon processes, electron-phonon and defects were estimated. The phonons scattering through roughness boundaries due to rough nanowires indicates a smaller phonon mean free path compared to that of their diameters. However, the Casimir limit for phonons mean free path particularly in 22nm nanowire diameter found to be due to phonons involved in completely diffused boundary scattering processes, while for other diameters (37, 56, 115) nm, the effects were smaller with values ranging from 0.35 to 0.685. In general, for a given temperature, LTC decreases with the decrease of NWs diameter**.**

KEY WORDS: Surface roughness, Lattice thermal conductivity, SiNWs, Debye-Callaway model
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1.INTRODUCTION :

Since the end of last century, low-dimensional substances have received a lot of interest for the benefit of electronic devices shrinkage and the necessary of thermoelectric applications[1, 2]. Low-dimensional materials are thought to have a higher potential factor due to their electron energy filtering and size-quantization effects [3, 4] as well as lower thermal conductivity [5, 6].

Roughness is the measurement of the physical surface of small scale variation in height. That is in contrast to large scale changes, it might be part of the surface's geometry[7]. Roughness is an unwanted characteristic since it may induce friction, wearing, drag, and heat loss. It causes significant losses and damages, particularly in the manufacturing industries that deal with heat exchangers. Li *et al* confirmed that thermal conductivity is low in smooth VLS-grown SiNWs[8]. Experimental results shows a rough surface for VLS-grown SiNWs having their root-mean-square values ranging from 0.3nm to 5nm [9].

However, electroless-etched (EE) SiNWs have a thermal conductivity that is five to eight times less than smooth VLS-grown SiNWs and the abnormally substantial decrease in LTC might be attributed to the surface roughness in EESiNWs[1]. Moore *et al.*, were used MC simulations and suggest a backscattering process in SiNWs due to sawtooth features[10]. The influence of surface roughness on LTC examined due to multi phonon scattering at a rough surface[11]. When the crystal layers are broken to produce a nanowire, a new type of deformation for the lattice is formed. This bends the surface structure resulting in additional modes of the lattice vibration, denoted by a Gruneisen parameter and that consequently reduces thermal conductivity. In this work attempts are made to examine the role of surface roughness on LTC in SiNWs with diameters of 115, 57, 37 and 22nm using modified Debye-Callaway model. Both of transverse and longitudinal phonon Gruneisen constants, Debye temperature, sample dimensions are all changeable factors in this model, especially surface roughness and surface stress. The mass-difference, phonon Umklapp, boundary, and

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phonon-electron, and other processes are often regarded as scattering mechanisms[12]. These scattering rates were adding together by using Matthiessen's rule. In addition to that, the change in the two boundary effects of phonon dispersion caused by spatial confinement, and non-equilibrium phonon distribution caused by partly diffuse border scattering were taken in the calculations. These effects correct the model in order to compute lattice thermal conductivity.

2- Calculation methods for LTC

The Debye-Callaway's formulation for LTC includes two parts $K_{DC}^{L(T)} = K^L + 2K^T$, for both longitudinal and transverse modes, where, $K^L = K_1^L + K_2^L$ and $K^T = K_1^T + K_2^T$ [13, 14] calculated as follow,

$$\left.\begin{aligned} K_1^{L(T)} &= \frac{1}{3}\frac{k_B^4}{2\pi^2\hbar^3 v_{L(T)}}T^3\int_0^{\frac{\theta_{L(T)}}{T}}\frac{\tau_C^{L(T)}x^4e^x}{(e^x-1)^2} \\ K_2^{L(T)} &= \frac{1}{3}\frac{k_B^4}{2\pi^2\hbar^3 v_{L(T)}}T^3\frac{\left[\int_0^{\frac{\theta_{L(T)}}{T}}\frac{\tau_C^{L(T)}x^4e^x}{\tau_N^{L(T)}(e^x-1)^2}\right]^2}{\int_0^{\frac{\theta_{L(T)}}{T}}\frac{\tau_C^{L(T)}x^4e^x}{\tau_R^{L(T)}\tau_N^{L(T)}(e^x-1)^2}} \end{aligned}\right\} \quad \ldots(1)$$

The ratio (1/3) is derived from the three vibration spectrum contribution branches, k_B is the Boltzmann constant, $\hbar$ is the Planck constant, ω is the frequency of phonon, and $v_{L(T)}$ are the longitudinal and transverse velocities for acoustic phonons, respectively and $x = \hbar\omega/k_BT$. In Eq.(1), $(\tau_N)^{-1}$ is the normal scattering rate while $(\tau_R)^{-1}$ is its addition of resistive scattering processes, denoted by $(\tau_C)^{-1} = (\tau_N)^{-1} + (\tau_R)^{-1}$ T and L are transverse and longitudinal phonons, respectively.

3- Phonon relaxation rates

To obtain LTC according to Eq.(1), the temperature and size dependent on scattering rate τ_C should be calculated. That is the processes not conserving the crystal momentum and known to contribute lattice thermal resistance[15]. The resistive scattering processes are boundary, dislocation, mass difference, three phonon Umklapp processes, normal phonon processes, as well as phonon-electron scattering. Matthiessen's formula is used to calculate the summation of phonons relaxation time by adding their inverse for various scattering mechanisms, in this case it is given as to the following equations;

$$(\tau_R^{L(T)})^{-1} = (\tau_U^{L(T)})^{-1} + (\tau_M^{L(T)})^{-1} + (\tau_N^{L(T)})^{-1} + (\tau_{Ph-e}^{L(T)})^{-1} + (\tau_B^{L(T)})^{-1} \quad \ldots\ (2)$$

$(\tau_U^{L(T)})^{-1}$ is the Umklapp resistance scattering calculated from the relation;

$$[\tau_U^{L(T)}(\omega)]^{-1} = \left(\frac{\hbar\gamma_{L(T)}^2}{Mv_{L(T)}^2\theta_D^{L(T)}}\right)\omega^2Te^{-\theta_D^{L(T)}/3T} \quad \ldots(3)$$

where $\gamma_{L(T)}$, $\theta_D^{L(T)}$ and $v_{L(T)}$ are longitudinal and transverse Gruneisen parameters, Debye temperatures and group velocities respectively.

The second term in Eq.(2), is scattering from isotopes (I_{Iso}) and impurities (I_{Imp}), they calculated according to;

$$[\tau_M^{L(T)}(\omega)]^{-1} = I\omega^4 = (I_{Iso} + I_{imp})\omega^4 \quad \ldots(4)$$

$$[\tau_M^{L(T)}(\omega)]^{-1} = \left(\frac{V_o}{4\pi v_{L(T)}^3}\Gamma_M + \frac{3V_o^2S^2}{\hbar v_{L(T)}^3}N_{imp}\right)\omega^4 = \left(\frac{V_o}{4\pi v_{L(T)}^3}\sum_i f_i(1-\frac{M_i}{\bar{M}})^2 + \frac{3V_o^2S^2}{\hbar v_{L(T)}^3}N_{imp}\right)\omega^4 \quad \ldots\ (5)$$

where f_i is the i^{th} atoms relative concentration, $\bar{M} = \sum_i f_i M_i$ is the mean atomic mass, M_i is the i^{th} impurity atom or defects mass, and Γ is the point-defects scattering strength measure. In this work, the contributions of vacancies, the anharmonicity due to host-impurity atom linkage, and the volume difference for the impurity atoms in Eq.(5) are ignored. However, these contributions are generally minor and may be adjusted through a simulation technique by increasing the mass difference effective concentration term.

The three main isotopes are 92% of Si^{28}, 4.9% of Si^{29}, and 3.1% of Si^{30}, their average atomic mass for Si is equal to 28.0855amu [16] . The third term in Eq.(2), representing the normal process and is calculated according to[17]:

$$[\tau_{N}^{L(T)}(\omega)]^{-1} = \left(\frac{k_B}{\hbar}\right)^{b} \left(\frac{\hbar\gamma^2 V^{(a+b-2)/3}}{MV^{(a+b)}}\right)\omega^{a}T^{b} \quad \ldots(6)$$

Hence a and b are adjustable parameters they are equal to 2, 3 and 1, 4 for both longitudinal and transverse phonons, respectively. The forth term which is the relaxation time rate denoted by $[\tau_{Ph-e}^{-1}(\omega)]$, is due to acoustic phonons which explain the low doping levels interaction between phonons and electrons, it can be expressed as;

$$[\tau_{Ph-e}^{L(T)}(\omega)]^{-1} = \frac{n_e\varepsilon^2\omega}{\rho v_{L(T)}^2 k_B T}\sqrt{\frac{\pi m^* v_{L(T)}^2}{2k_BT}}\, e^{\left(\frac{-m^* v_{L(T)}^2}{2k_BT}\right)} \quad \ldots(7)$$

where n_e is the conduction electrons concentration, ε is the deformation potential, ρ is the mass density, and m^* is the electron effective mass. It is assumed that phonons confinement does not strongly affects the phonon-electrons scattering rates [18].

The Casimir length (L_C) for a completely rough specimen is used to calculate the scattering rate from phonon–boundaries, which is supposed to be independent on the frequency and temperature. To ensure the model's consistency, the formulation of the relaxation from boundary scattering was altered by adding the parameter P and length l into the semi equation.

$$[\tau_{B}^{L(T)}(\iota, P)]^{-1} = v^{L(T)}\left[\frac{(1-P)}{Lc(1+P)} + \frac{1}{\iota}\right] \quad \ldots(8)$$

This introduce the condition of specular and diffuse boundary scattering at the interfaces. Hence P describe the effects of interface roughness on phonon boundary scattering, it denotes the probability for the surface specular phonon or diffuse scattering (1-P). When P=1, the scattering is purely specular scattering, consequently there will be no effect of boundary scattering on the process of heat conductivity. In the case of this work a rod of radius R, $L_C=2R$, and (l) the length of the sample found to be 3.8mm for the bulk state of Si and is used in this work[19].

Accordingly, lattice thermal conductivity for the bulk silicon is obtained, through the best fit to that of the experimental data as shown in Fig.1. Table 1 lists all of the material properties utilized in the LTC computation[20] .

For nanowires, several related parameters in Eq.(1) are modified according to the sample size dependence such as, Debye temperatures $\theta_D^{L(T)}$ and group velocity $v_g^{L(T)}$ for both their branches of longitudinal and transverse phonon modes, respectively. Their values were evaluated depending on the melting point formula, as follow[21, 22]:

$$\frac{T_m^n(r)}{T_m^B(\infty)} = \left(\frac{V(r)}{V(\infty)}\right)^{\frac{2}{3}} e^{\left(-\frac{2(S_{m-R})}{3R\left(\frac{r}{rc}\right)-1}\right)} \quad \ldots(9)$$

Where R is the ideal gas constant it has the value of 8.31J.mol^{-1}.K^{-1}, S_m is bulks melting entropy for Si its equal to 30J.mol^{-1} K^{-1}[23], r_c refers to a critical radius that is all the atoms forming the particle are located on its surface, its value can be obtained from, r_c=(3-d)h. hence h denotes the first surface layer height and is calculated according to [21],[22];

$$h = 1.429d_o \qquad 10)$$

where d_o is mean bond length, calculated from $d_o = \sqrt{3}a/4$, for Si, h has the value of 0.3361nm[24]. For low-dimensional crystals, r_c

depends on the dimension of the structure denoted (D): where D = 0,1, and 2 for nano particles, wires and films respectively[24]. Size dependence Debye temperature (θ_D^n) and phonon group velocities (v_g^n) in nanowires were calculated from the following proportional relation [19].

$$\frac{T_m^n(r)}{T_m^B(\infty)} = \frac{v_g^n(r)}{v_g^B(\infty)} = \frac{\theta_D^n(r)}{\theta_D^B(\infty)} \quad (11)$$

Where v_g, θ_D and T_m are group velocity, Debye and melting temperature for the bulk that is denoted by B and nanowires denoted by n, respectively. Their values with that of size dependence are stated in table 2.

In this work, the modified Debye-Callaway model due to the surface effects were used to calculate LTC in silicon nanowire diameters of 22, 37, 56, and 115nm. The process was depending on effects of both interface roughness and surface stress on scattering from phonon by boundary within the existence due to all other scattering types. The total LTC of nanowires can then be expressed by[18];

$$K_{tot}^{L(T)}(T,P) = K_{DC}^{L(T)}(T,P) - \Delta K_{wire}^{L(T)}(T,P) \quad \ldots(12)$$

The first term $K_{DC}^{L(T)}(T,P)$ is the Debye-Callaway model before modification as mentioned above, and $\Delta K_{wire}^{L(T)}(T,P)$ is the deviation due to their phonons redistribution caused by the effects of boundary scattering with that of the interface roughness, and have the following form;

$$\Delta K_{wire}^{L(T)}(T,P) = 12\left(\frac{k_B T}{\pi\hbar}\right)^3 \left(\frac{k_B}{V}\right) \int_0^{\frac{\theta_D}{T}} \frac{\tau_c x^4 e^x}{(e^x-1)^2} G^{L(T)}[\eta(x),P]\,dx \quad \ldots(13)$$

Hence, η, calculated from;

$$\eta(x) = d / \lambda(x) \quad \ldots(14)$$

where d is the wires diameter and λ(x) is the phonon mean free path, it is calculated from $\lambda(x) = v_g(x)\tau_c(x)$, and obtained from $G[\eta(x), P]$, given by the following:

$$G^{L(T)}[\eta(x),P] = (1-P^2)\sum_{j=1}^{\infty} jP^{j-1}\int_0^1 (1-y^2)^{1/2} S_4(j\eta y)\,dy \quad \ldots(15)$$

The parameter *G* in this equation depends on the shape of the wire section and its characteristic ratio to λ(x). $S_n(u)$ which is the roughness influence on phonon-boundary scattering is calculated from;

$$S_n(u) = \int_0^{\pi/2} e^{-u/\sin\theta} \cos^2\theta \sin^{n-3}\theta\, d\theta \ldots (16)$$

By Substituting Eqs.(13 to 16) in Eq.(12), the expression for $K_{tot}^{L(T)}(T,P)$ can be simplified to

$$K_{tot}^{L(T)}(T,P) = \left(K_{DC}^{L}(T,P) - \Delta K_{wire}^{L}(T,P)\right) + 2\left(K_{DC}^{T}(T,P) - \Delta K_{wire}^{T}(T,P)\right) \quad \ldots(17)$$

This equation, is used to calculate the effects of surface roughness on LTC in SiNWs interested in this work. The fitting parameters for all the cases considered in the calculations given in table 2 and Fig.2.

4. Analysis of Results

Calculated lattice thermal conductivities for wires having diameters ranging from 22 to 115nm with these reported of experimental data are shown in Fig.2. Calculations were performed by using values of a, ρ, Γ, m^*,ε for both bulk and NWs from Table 1, and values of, P, g , and N_{imp} (this is seen in Table 2) as adjustable parameters are used in table 2.

The likelihood of specular reflection (P) at the lateral boundary varies with temperature. In the case of randomly distributed surface roughness with a Gaussian distribution, the specularity parameter(P) is calculated by using Ziman's formula [25] as [$P=\exp(-16\pi^3\eta^2/\lambda^2)$], η is the root mean square surface roughness, λ is the phonon wavelength. In high temperatures, the dominant phonon wavelength decreases and atom movement on the lateral boundaries increases, resulting in an increase in root mean square surface roughness. As a result, the probability of specular reflection is diminishing, and leads to an increase of diffuse scattering, as shown in Fig.3. And their values are given in table 2.

Thermal conductivities for a fully specular reflections at lateral limits as P=1 is independent on diameter and has the same thermal conductivity of bulk silicon so that ΔK_{wire} decreases. Since raising P reduces the significance of boundary scattering, the influence of boundary like surface stress become less relevant. As shown in previous examples when P is less than one, the LTC for SiNWs rises with the increase diameter, and their dependency is more pronounced smaller values of P.

The mean root square deviation of surface height from the reference plane η is calculated from $\eta=(1-P)D/10$, and their dependence on nanosize is given in Fig.4[26]. According to this figure, surface roughness that increase in smaller nanosize is corresponds to the higher probability of diffuse scattering, and decrease s the LTC as indicated in Fig.2.

Since all these crystal imperfections are then remaining the same for all the nanowires diameter except lattice dislocation, then it's from the fitting process is obtained and drawn with size as shown in Fig.5. However, lattice dislocation affects to decrease LTC in the left hand side of the LTC peak maximum, while impurities were on its right side. The dislocation concentration increase moves the peak point temperature to its right side[27].

At high temperature, ($T<\theta_D$), phonon-phonon scattering plays an important role in restricting thermal conductivity[28], and its affects strongly by lattice anharmonicity denoted by the Gruneisen parameter (γ). According to Fig.6 the increase of γ for smaller nanowires reflects the increase of lattice anharmonicity and according the decrease of LTC.

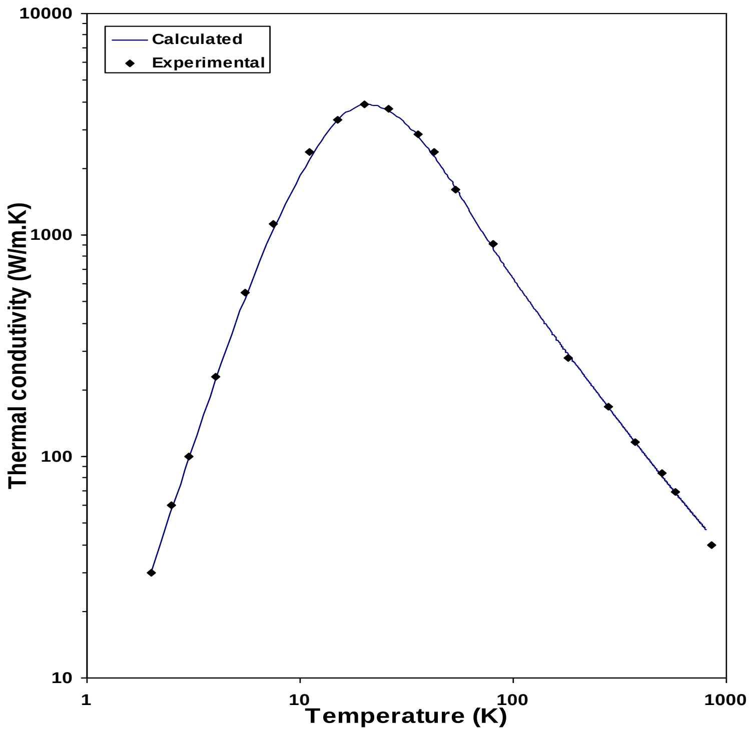

Fig.1: Temperature dependence of lattice thermal conductivity for bulk Si compared to that of the reported experimental data[17].

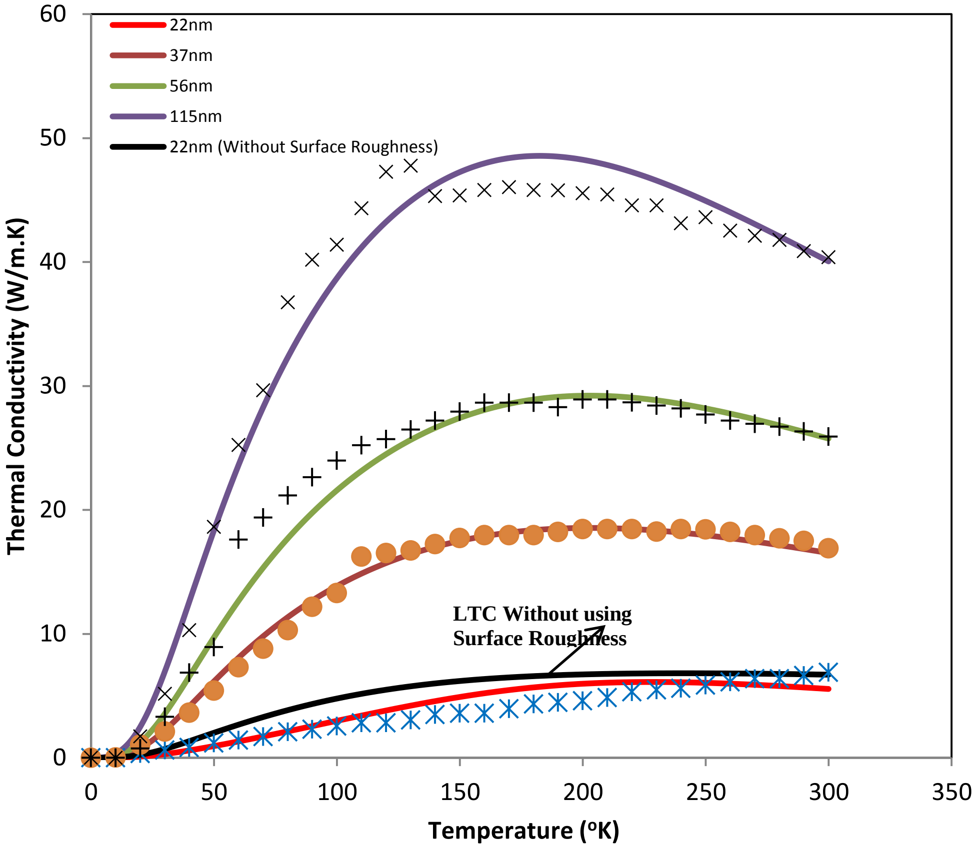

Fig. 2: Thermal conductivity calculated of SiNWs with various diameters.

Table 1: Basic parameters used to calculate phonon scattering rate in both bulk state and nanowires of Si.

Parameters	Values
Lattice constant a (A^o)	5.5431
Atomic mass M (Kg)	46.6×10^{-27}
Crystal density ρ($Kg.m^{-3}$)	2.33×10^{3}
The mass-difference scattering strength Γ	2.0024×10^{-4}
Electron effective mass $m^*(m_o)$	0.26
Deformation potential ε (eV)	9.5

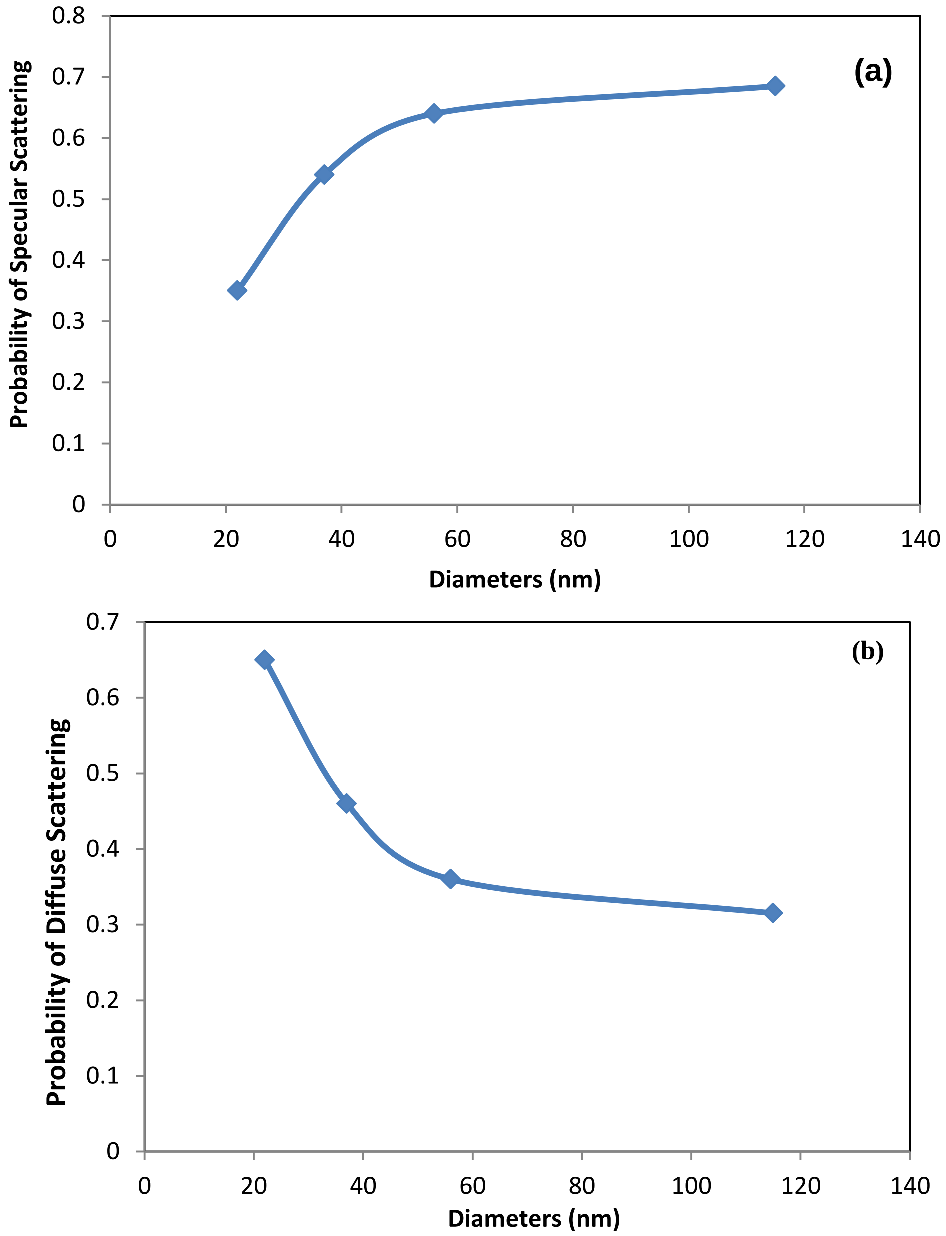

Fig. 3: Variation of probability of (a) specular scattering, (b) diffuse scattering on the surface with diameters.

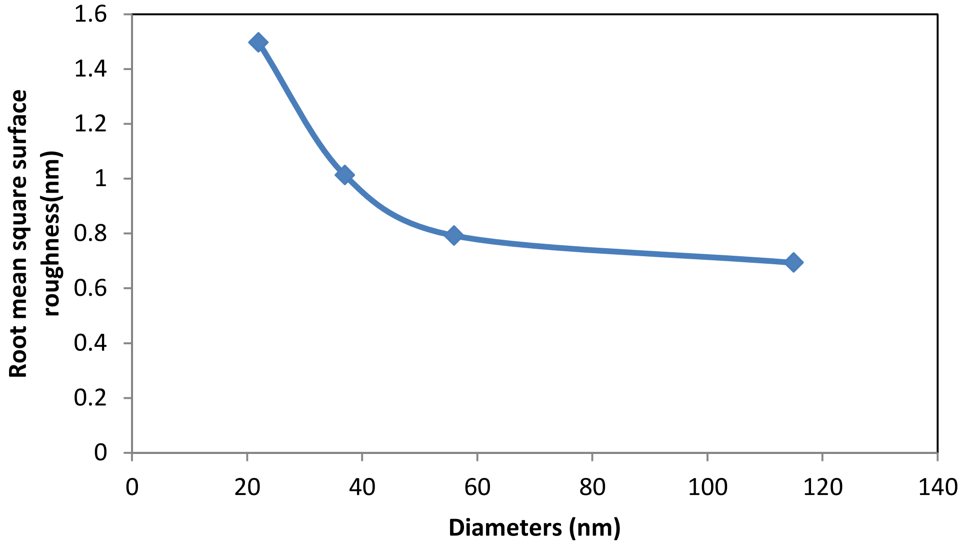

Fig. 4:Variation the root mean square surface roughness with diameters for 22nm to 115nm.

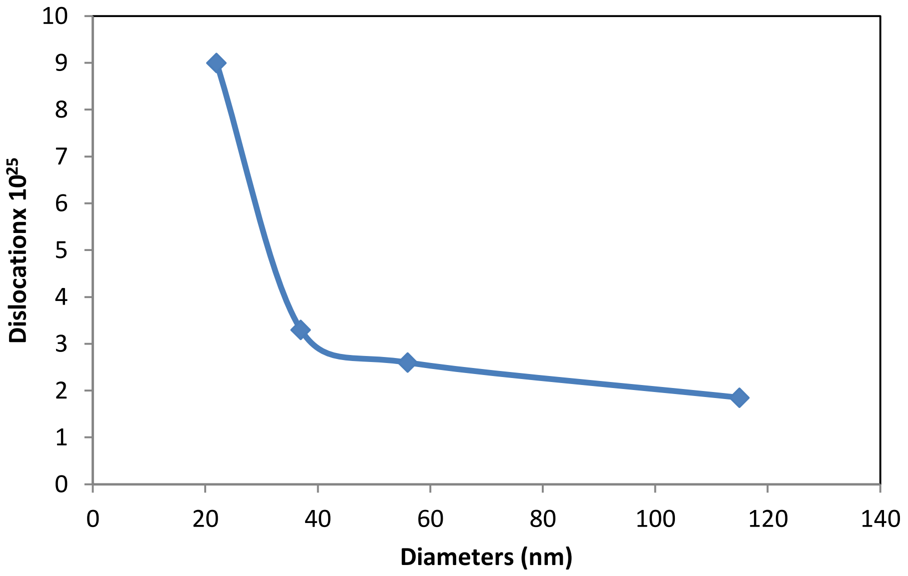

Fig. 5: Variation of dislocation with size.

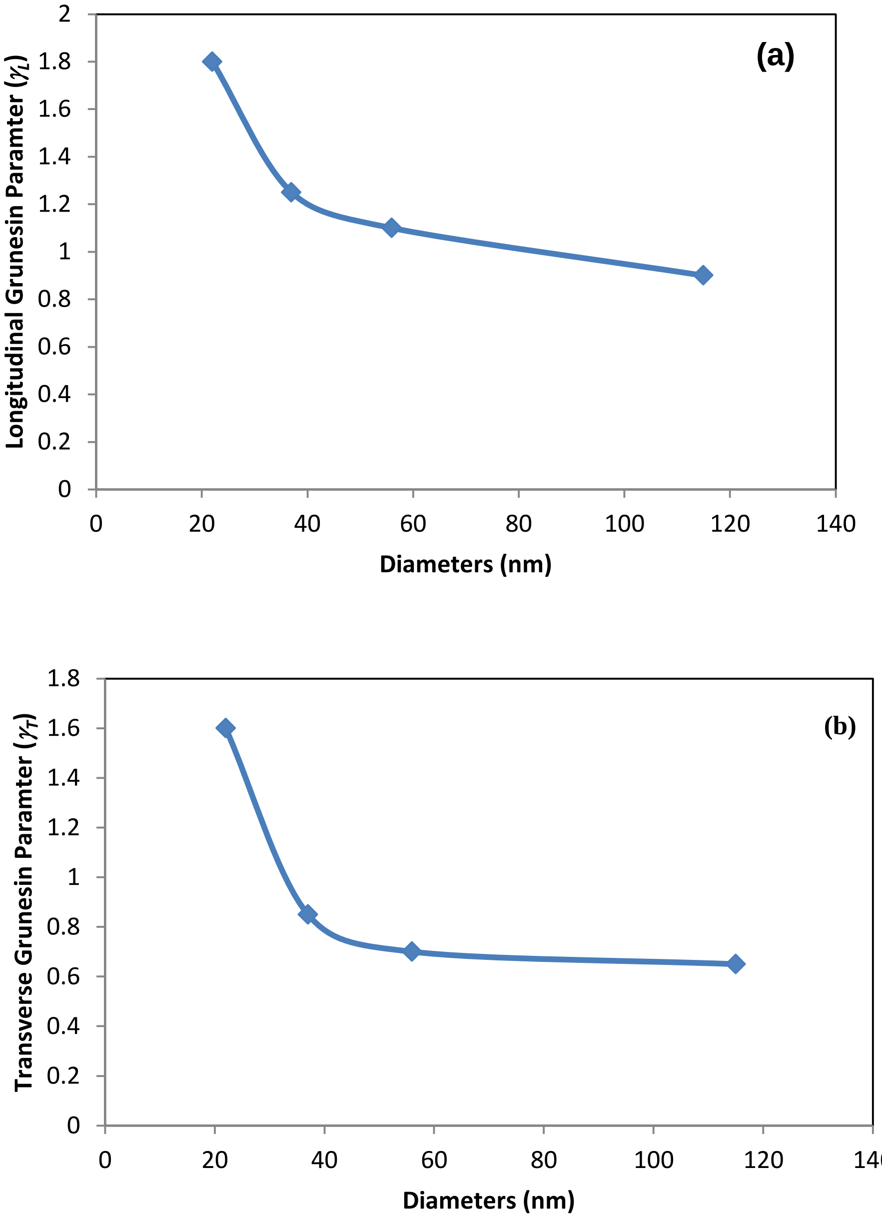

Fig. 6: Variation of Longitudinal and transverse Gruneisen with diameters.

Table 2: Parameter values from Eqs.(9-11) for different diameter for silicon nanowires.

Diameter (nm)	Melting point T_m (K)	Debye temperature θ_D (K)		Group velocity v_g x 10^3 (m/sec)	
		θ_D^L	θ_D^T	v_g^L	v_g^T
Bulk	1690	586	240	8.47800	5.850
115	1658	580.041	237.560	8.39179	5.791
56	1620	573.678	234.954	8.29974	5.727
37	1583	567.220	232.309	8.20630	5.663
22	1510	553.967	226.881	8.01456	5.530

Table 2: The fitting parameters of SiNWs used in calculating LTC.

Diameters(nm)	Probability Scattering Due to Surface Roughness		Grunesin parameters (γ)		Dislocation x 10^{25} N_{imp}
	P	1-P	Longitudinal	Transverse	
22	0.35	0.65	1.8	1.6	9
37	0.54	0.46	1.25	0.85	3.3
56	0.64	0.36	1.1	0.7	2.6
115	0.685	0.315	0.9	0.65	1.85

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37	0.54	0.46	1.25	0.85	3.3
56	0.64	0.36	1.1	0.7	2.6
115	0.685	0.315	0.9	0.65	1.85

5. Conclusion

Surface influences a clear effect on heat transfer in one-dimensional SiNWs particularly for smaller size such 22nm diameters. It has been proven empirically as well as analytically that increasing roughness due to the diameter reduction can significantly lower lattice thermal conductivity.

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Author Contributions *H. T. TAHA* introduced the editing and writing the manuscript and supervised the project.
E. A. MOHAMMED performed the computations.
Availability of Data and Material The data associated with a paper is available, and under what conditions the data can be accessed.

Statement and Declarations
We confirm that the manuscript has been read and approved by all named authors and that there are no other persons who satisfied the criteria for authorship but are not listed. We further confirm

that the order of authors listed in the manuscript has been approved by all of us.

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