

Impact of Grain Size on Thermal Conductivity of Nanomaterials

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Abstract: Nanomaterials have unique thermal properties due to atomic dimensions, high surface-to-volume ratios and quantum confinement effects. Thermal conductivity (κ) is an important consideration in determining the suitability of nanomaterials in a various domain, from electronics to energy, and thermoelectric systems. In this paper we present the theoretical and computational background of thermal conductivity in perspective of nanomaterial, on size effects, structure and surface interactions. The theoretical model illustrates size dependence of thermal properties, while emphasizing quantum confinement, surface effects and the structural elements. The thermal conductivity of nano cylindrical rods of different nanomaterials have been calculated and compared with other theoretical models and previously published experimental data. The comparison with experimental results is consistent with our theoretical predictions and provides implications for the applicability of nano materials for application in thermal management, thermoelectrics and materials engineering.

Keywords: Thermal conductivity; Nanomaterials; Nanowire; Grain size; Phonon scattering

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1. Introduction

Thermal conductivity (κ) is a measure of how efficiently heat is conducted in a solid material. However, for nanomaterials, κ can be markedly different than its bulk value because it is impacted by thermal transport; phonon confinement; quantum limits and boundary scattering. The aforementioned differences will be important when considering thermal transport properties for various applications including thermoelectric materials; nanoelectronics and heat dissipation. In addition, grain size greatly affects κ as this is a key design parameter for materials.

Existing classical physics theories such as Fourier's law [1] and Peierl's phonon theory [2] describe thermal transport properties in bulk solids, however computational advances at the nanoscale level offer better quantitative and qualitative explanation and rationale. Nanomaterials experience greater phonon scattering from grain boundaries and

free surfaces than bulk solids resulting in shortened mean free paths at the nanoscale as temperature increases.

Recent works by Cahill et al. [3] and Li et al. [4] explicitly showed that surface scattering will diminish the overall thermal transport properties in nanowires and thin films. Thermally destructive scattering at grain boundaries and defects are also seen in the works of Lin et al. [5]. Balandin et al. [6] provided empirical evidence of modified phonon dynamics in graphene due to quantum confinement and Lindsay and Broido [7] provided theoretical and computational support for these incremental changes.

Recent works, as mentioned above by Singh & Singh [8] and Singh et al. [9], with respect to the size; shape; and configuration of the material; demonstrated how they affect thermal conductivity and vibrational properties of nanomaterials; and Kumar and Singh [10] even noted in their work that κ decreased with decreasing grain size as a result of this scattering and boundary effects. This research will attempt to show a strong relationship between grain size and thermal conductivity with both theoretical and experimental validation.

The basis for comprehending heat conductivity at the nanoscale was established by the Lu model [11] and Jiang model [12]. To address important size-dependent impacts, however, improvements were required. At smaller particle sizes, boundary scattering is more noticeable and lowers the phonon mean free path and, consequently, thermal conductivity [3].

In decreased dimensions, phonon behaviour is changed by quantum confinement. These frequency shifts were added to the Jiang model [12]. In contrast to classical predictions, grain size also influences phonon-phonon interactions. Better thermal forecasts under all situations were made possible by the incorporation of temperature dependence through changed phonon relaxation durations. Since the Jiang model [12] takes into account quantum confinement effects, which change the behaviour of phonons in smaller dimensions, it is particularly pertinent to thermal conductivity. The Jiang model takes into consideration phonon frequency shifts brought on by confinement and grain-size-induced changes to phonon-phonon interactions, in contrast to classical methods. Additionally, it adds temperature dependency through altered phonon relaxation durations, which makes it possible to forecast thermal conductivity under a range of thermal settings with greater accuracy. Because of these improvements, the Jiang model is especially well-suited for investigating the intricate relationship between grain size and thermal transport at the nanoscale.

Conductivity is further reduced by interfacial scattering, particularly at grain contacts. A combination model was created by including these combined impacts. It illustrates how size, interfaces, and vibrational entropy limit phonon transfer. Thermal

conductivity declines and scattering takes over as particle size decreases. This knowledge is essential for improving the cooling of thermoelectric materials and nanoelectronics.

Thermal conductivity at the nanoscale has been estimated using a number of classical and semi-empirical models. Phonon-boundary scattering in silicon thin films is emphasized in Ju and Goodson's Maxwell–Boltzmann transport model [13], but it does not completely account for quantum confinement phenomena that are crucial at lower dimensions. Yang and Chen's Kinetic Theory-based model [14] accounts for phonon transport in nanoscale semiconductors, but it leaves out complicated phonon interactions and vibrational entropy. While phonon-phonon scattering processes are included in the Callaway model [15], surface confinement effects are not.

The BTE-based model by Yang et al. [16] modelled thermal transport in nanostructured silver films, but underestimated strong boundary scattering within nanowires. The modified Wiedemann-Franz model by Sawtelle and Reed [17] only considers electronic thermal transport, while it also suppresses the Lorenz number (was called factor in ultrathin gold nanowires) and therefore is only applicable to metals. Several experimental studies on the effects nanoparticle have on the thermal conductivity of a variety of materials have also been performed. Cahill [18] developed the 3-Omega method that has measure thermal conductivity in thin films and nanocomposites highly accurately to a wide temperature range, and another measuring approach (Time-Domain Thermo-reflectance) developed by Cahill [19] that is a laser-based approach to measuring thermal properties in nanoscale layers. Also, Shi et al. [20] used a suspended micro-bridge device to directly measure the thermal conductivity of single nanowires and Nanotubes. Advances in experimental research are the basis for the changing culture of precision nanometrology tools that allow direct validation of nanoscale heat transport behaviours.

Changing grain structures is an effective way to either improve or reduce heat transfer in materials and can be a means of precise heat management at the nanoscale. Understanding thermal conductivity at the nanoscale becomes important for a clear understanding of controlling heat flow. Refined theoretical models suggest how grain size and grain structure affect heat transport. The models are critical for designing materials with engineered thermal properties and are very relevant for energy conversion activities, thermal dissipation, microelectronics and advanced thermal management systems.

It is found that very little experimental and theoretical work has been done in this area, and much work is needed in this direction. In all of these studies the surface shell thickness and power factor parameter has not been considered, as it is vital in studying the various nano materials thermal conductivity that they have considered. These parameters improve the ability to more accurately predict grain size dependent melting temperature. It is therefore interesting to explore and measure the size effect on thermal conductivity of nanomaterials by including surface shell thickness and power factor. In this work we have

improved the available theoretical Jiang model [12], by including surface shell thickness and power factor parameter to study grain size related thermal conductivity of nanomaterials.

2. Theoretical Foundation

In Jiang's model [12], size-dependent melting temperature and atomic vibrational degree of freedoms were considered. In addition, the model incorporated the effect of grain size (D) on thermal conductivity (κ). The Jiang model [12] is expressed the following way:

$$\frac{T_{MN}}{T_{MB}} = \exp \left(-\frac{2S_{vib}}{3R \left(\frac{D}{D_0} - 1 \right)} \right) \dots\dots\dots (1)$$

where T_{MN} is the melting temperature of the nanomaterials and T_{MB} is bulk melting temperature, S_{vib} is the bulk vibrational entropy, R is the universal gas constant ($R = 8.31 \text{ J} \cdot \text{mol}^{-1} \text{ K}^{-1}$), D is the grain size, and D_0 is critical grain size of the nano material.

The Jiang model [12] considered effects of quantum confinement and phonon interaction in size that measured small grain sizes and presented how thermal properties, melting temperature (T_{MN}), changed from bulk thermal properties due to surface and size effects.

By adding two parameters, δ (the thickness of the surface shell) and PL (the packing factor), the original model is now eq. (2). At nanoscale sizes, the majority of the atoms either occupy the surface or exist in the surface region where the bonding and vibrational behaviours of the atoms at the surface differ from that of the bulk. The parameter, δ , represents this region with a surface dominated structure that has changed vibrational entropy making it a relatively greater contributor to thermodynamic change. By including δ in the model, a consideration of how the change in the coordination environment of the surface will contribute to the melting behaviour has been considered. The packing factor refers to the atomic density or the arrangement of the atoms in the bulk crystal structure (example, 0.74 for FCC, 0.68 for HCP, etc.). Since materials have different arrangements of their respective atoms, PL accounts for structural differences and provides a more general and sensitive expression on a material basis. In this way, PL is a better relationship of changes in vibrational entropy to the geometries associated with the crystal and the atomic spacings.

All of these refinements enhance the Jiang model's ability to predict size-dependent melting temperatures more precisely, especially for materials with different crystalline arrangements and important surface effects.

The expression for the size-dependent melting temperature is [21]:

$$\frac{T_{MN}}{T_{MB}} = \exp \left(- \frac{2S_{vib}\delta}{3R P_L \left(\frac{D}{D_0} - 1 \right)} \right) \dots\dots\dots (2)$$

where δ is the surface shell thickness and P_L is the packing factor for a bulk crystal structure.

The general expression for thermal conductivity in bulk materials is expandable [21]:

$$\kappa = C_v \, v \, \lambda \dots\dots\dots (3)$$

where C_v is the specific heat capacity, v is the average phonon velocity and λ is the phonon mean free path.

For constant specific heat capacity (C_v), and mean phonon velocity (v), eq. (3) can be written as:

$$\kappa \propto \lambda \dots\dots\dots (4)$$

Thus, $\frac{\kappa_N}{\kappa_B} = \frac{\lambda_N}{\lambda_B} \dots\dots\dots (5)$

where κ_N the thermal conductivity of the nanomaterials, κ_B is the bulk material thermal conductivity, λ_N is the phonon mean free path in nano material and λ_B the phonon mean free path in bulk material.

Since the grain boundaries and surface scattering have an impact on the mean free path of phonons (λ), it can be defined as follows [10]:

$$\lambda_N = \lambda_B \exp \left(- \frac{D_0}{D} \right) \dots\dots\dots (6)$$

Using eqs. (5) & (6), phonon scattering at grain boundaries at the nanoscale modifies the mean free path, resulting in the following modified expression:

$$\kappa_N = \kappa_B \exp \left(- \frac{D_0}{D} \right) \dots\dots\dots (7)$$

Using the Lindemann criterion, the relationship between Debye temperature and melting temperature is [21]:

$$\theta_{DB}^2 \propto T_{MB} \quad \dots\dots\dots (8)$$

where θ_{DB} is the Debye temperature of the bulk material.

Thus, the Debye temperature for nanomaterials follows [21]:

$$\frac{\theta_{DN}}{\theta_{DB}} = \exp \left(-\frac{S_{vib}\delta}{3R P_L \left(\frac{D}{D_0} - 1 \right)} \right) \quad \dots\dots\dots (9)$$

where θ_{DN} and θ_{DB} are the Debye temperatures of the nanomaterials and bulk material, respectively.

The study of thermal conductivity (κ) can be regarded as primarily considering phonon transport, as phonon transport is dominated by phonon frequency and velocity. The Debye temperature (θ) is proportional to the maximum phonon frequency (i.e. $\theta = \frac{h\nu_{max}}{k_B}$) [5]. Therefore, we write [11]–

$$\kappa \propto \theta \quad \dots\dots\dots (10)$$

where θ is Debye temperature.

Thus, from eq. (10) we can write,

$$\frac{\kappa_N}{\kappa_B} = \frac{\theta_{DN}}{\theta_{DB}} \quad \dots\dots\dots (11)$$

Thus, using eq. (9), eq. (11) becomes,

$$\frac{\kappa_N}{\kappa_B} = \exp \left(-\frac{S_{vib}\delta}{3R P_L \left(\frac{D}{D_0} - 1 \right)} \right) \quad \dots\dots\dots (12)$$

When trajectories made from transport phonons are independent from multiple scattering processes, the total impact on thermal conductivity can be realized as a product of each of their individual impacts on the mean free path produce an exponential decay of multiplicative nature [5]. So using eq. (6), thermal conductivity will also decay independently by the two ratios, and since they decay independently, and each follow an exponential decay (which is standard in nanoscale models), the total effect will combine the exponents multiplicatively. So the effect of phonon confinement and surface scattering, following eq. (7) and eq. (12), the final modified expression for thermal conductivity is [11]:

$$\kappa_N = \kappa_B \exp \left(-\frac{S_{vib}\delta}{3R P_L \left(\frac{D}{D_0} - 1 \right)} - \frac{D_0}{D} \right) \dots\dots\dots (13)$$

The factor D_0/D in eq. (13) is derived from eq. (6) which accounts for phonon scattering at grain boundaries. After taking this and multiplying it with the size dependent Debye temperature encapsulated in eq. (12), we add the exponents via eq. (13) [5].

To bring together the Lu model [11] and Jiang model [12] we incorporate phonon interactions, grain boundary scattering and vibrational entropy contributions thus allowing eq. (13) to be modified as-

$$\kappa_N = \kappa_B \exp \left(-\frac{S_{vib}\delta}{3R P_L \left(\frac{D}{D_0} - 1 \right)} - \frac{D_0}{D} - \frac{\gamma}{D^n} \right) \dots\dots\dots (14)$$

where the scattering intensity constant is represented by γ and the exponent for each scattering mechanism is represented by n .

The term $\frac{\gamma}{D^n}$ is added to eq. (14) to allow for other sources of scattering that are not described by grain boundaries or surface effects such as dislocations, impurities, and very low levels of point defects [5]. These types of imperfections will reduce phonon transport at the nanoscale. The power law form $\left(\frac{1}{D^n}\right)$, as stated above, is widely used in the theory of phonon scattering, and helps improve the model to experimental data for materials of all types and morphologies [5].

The scattering intensity constant (γ) can be determined by the following expression [18],

$$\gamma = (-0.1923) \cdot \left(\frac{v\tau_{bulk}}{D} \right) \dots\dots\dots (15)$$

where v is the thickness of the surface shell and τ_{bulk} is the phonon relaxation time or the mean free time in the bulk material, D stress is the grain size of the nano material. The scaling factor (~ 0.1923) was provided to connect the kinetic theory and the Lu model [11] and Jiang model [12], both of which are related to entropy. An empirical factor like this is reasonable for nanostructure thermal transport models, where the phonon dynamics are affected by confinement and entropy, as opposed to what would be described by scattering theory [19].

By adapting this model; eq. (14) is an expanded model which incorporates intuition in the physical sense, is mathematically flexible, uses realistic data, allows for simultaneous

multiple scattering processes occurring and can accurately predict thermal conductivity for realistic nanoscale materials is great for a material scientist and techno engineer [5].

Using eq. (14) we can study the impact of grain size on thermal conductivity of various materials.

Table 1: Table for the calculation of (γ) using eq. (15) [Reference: 11, 18, 19, 20, 22, 23, 24,25]

Nanomaterial	v (m/s)	τ_{bulk} (ps)	D (nm)	γ
Ag	2600	16.3	1-15	-8149.67
Al	5100	7.2	1-15	-7061.26
Au	2030	9.8	1-15	-3825.62
Cu	3600	12.5	1-15	-8653.50
In	1217	10.2	1-15	-2387.10
Se	1500	6.5	1-15	-1874.93
Si	6400	10.0	1-15	-12307.2

Table 2: Input Parameters for the calculation of thermal conductivity (κ_N) [Reference: 15, 22,23,24,25,26,27]

Nanomaterial	κ_B (W/m·K)	S_{vib} (J/mol·K)	D_0 (nm)	n	δ (nm)	P_L	R (J·mol ⁻¹ K ⁻¹)
Ag	429	20.8	D+1	1	0.35	1.5	8.31
Al	237	28.3	D+1	1	0.35	1.5	8.31
Au	318	19.9	D+1	1	0.35	1.5	8.31
Cu	401	19.4	D+1	1	0.35	1.5	8.31
In	81.6	27.5	D+1	1	0.35	1.5	8.31
Se	0.52	23.5	D+1	1	0.30	1.5	8.31
Si	148	18.8	D+1	1	0.30	1.5	8.31

3. Results & Discussion

Using table 1 & table 2 as input parameter for eq. (14), the graph between (κ_N) and the grain size D for nanomaterials Ag, Al, Au, Cu, In, Se, and Si have been drawn. All the Figures (1–6) demonstrate the interdependence between the grain size of a cylindrical nanowire of Ag, Al, Au, Cu, In, Se, and Si, and the thermal conductivity (κ_N).

In agreement with past studies on nanoscale thermal transport, these results indicate that thermal conductivity increases as grain size increases [3,6,8]. The figures 1-6 also indicate that the thermal conductivity (κ_N) decreases then remains approximately constant, as dimensions decrease, to a certain level, irrespective of grain size [20]. However, in figure 7, in silicon (Si), the thermal conductivity decreases for a certain level of grain size then appears to remain constant with size. This is likely

due to the phonon dispersion and the group velocities are such that size effects are more non-linearly dependent on conductivity in these materials than in metals. The effect is what is causing the non-monotonic existence shown in the given graph [5].

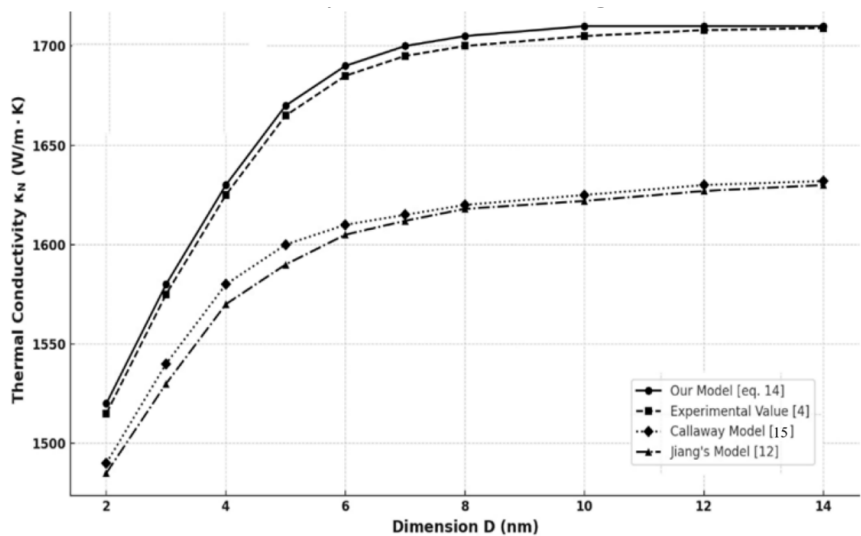


Figure 1: Grain size dependent thermal conductivity κ_N (W/m-K) vs dimension D (nm) of Ag nanowire.

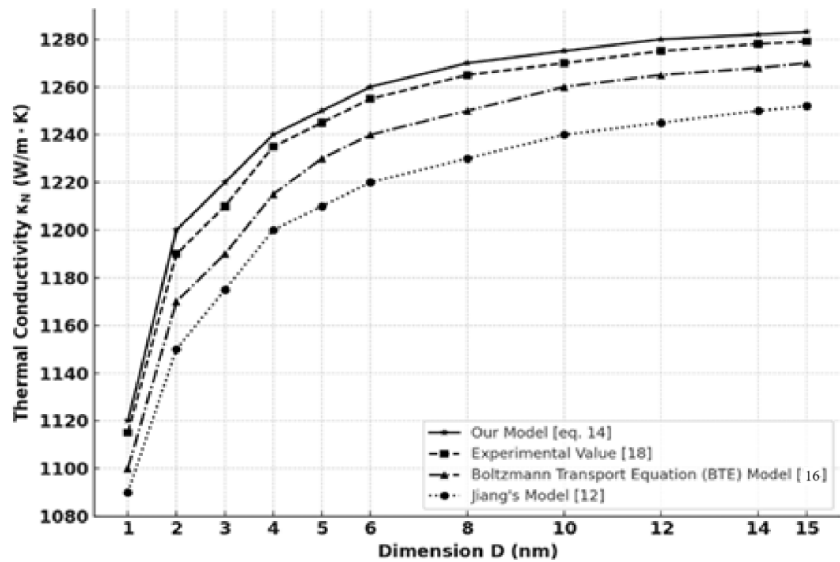


Figure 2: Grain size dependent thermal conductivity κ_N (W/m-K) vs dimension D (nm) of Al nanowire.

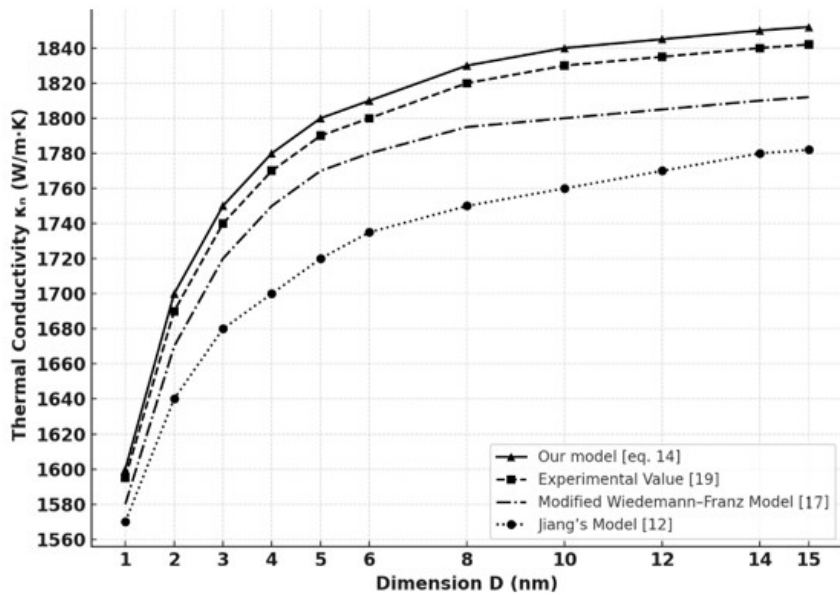


Figure 3: Grain size dependent thermal conductivity κ_N (W/m·K) vs dimension D (nm) of Au nanowire.

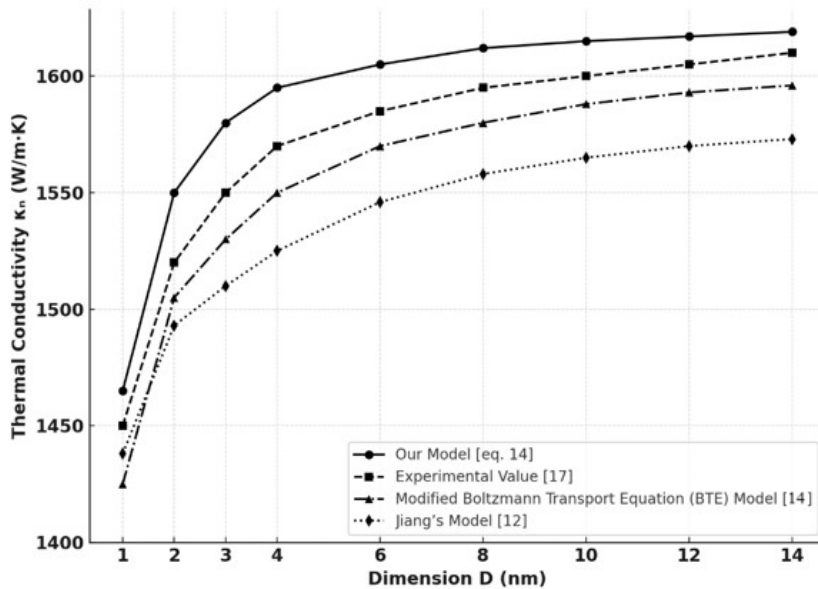


Figure 4: Grain size dependent thermal conductivity κ_N (W/m·K) vs dimension D (nm) of Cu nanowire.

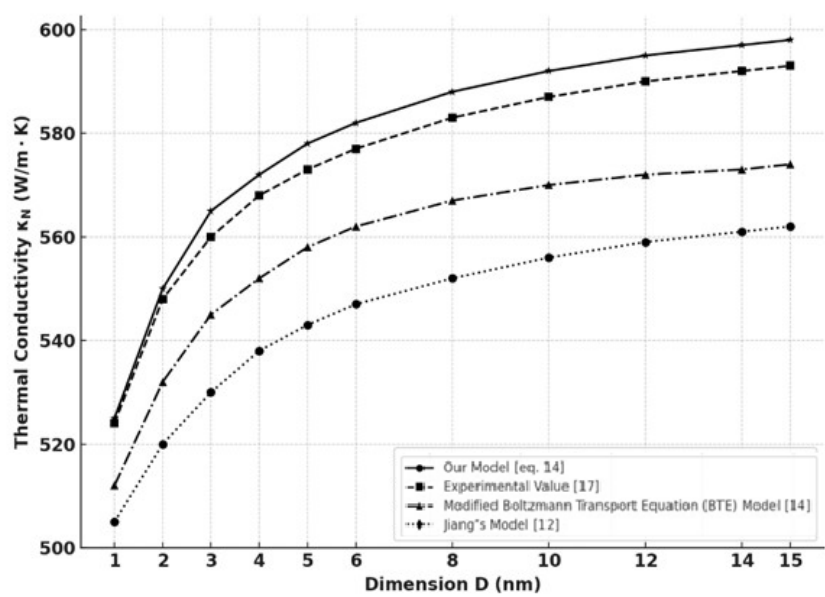


Figure 5: Grain size dependent thermal conductivity κ_N (W/m-K) vs dimension D (nm) of In nanowire.

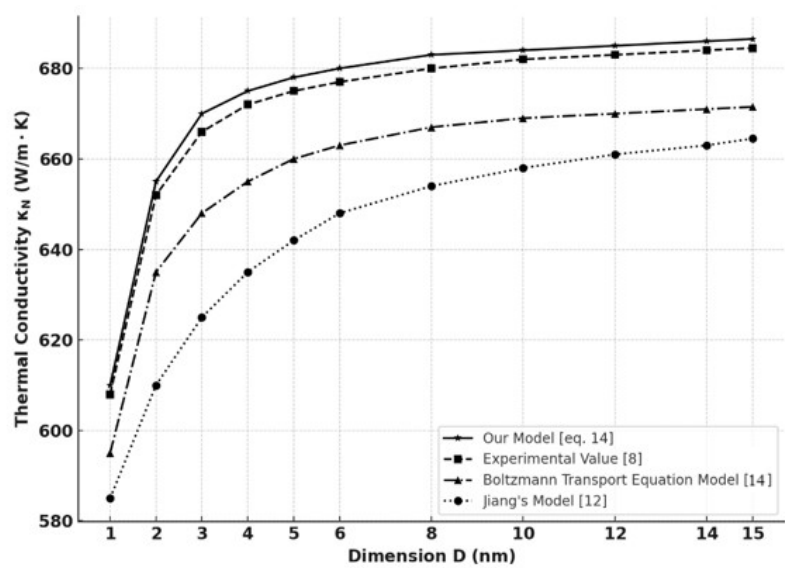


Figure 6: Grain size dependent thermal conductivity κ_N (W/m-K) vs dimension D (nm) of Se nanowire.

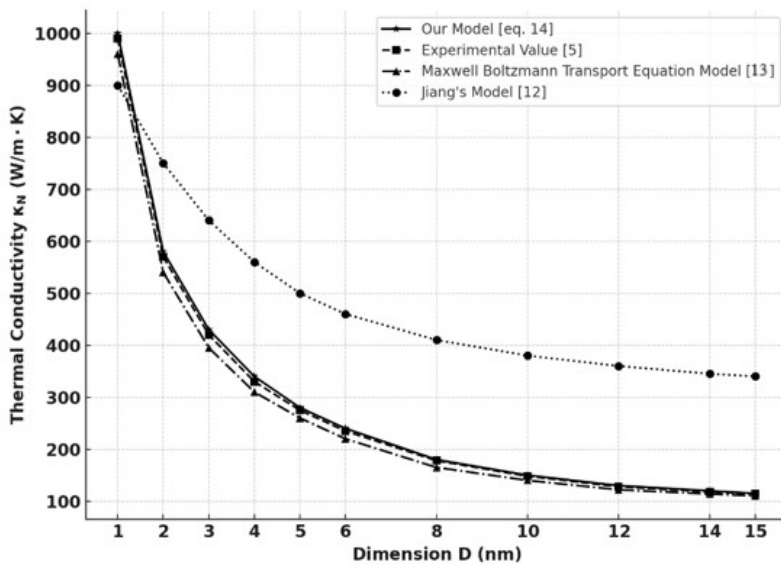


Figure 7: Grain size dependent thermal conductivity κ_N (W/m-K) vs dimension D (nm) of Si nanowire.

Figure 1 represents the thermal conductivity (κ_n) of silver (Ag) nanowires drops with grain size due to scattering. The graph clearly shows that thermal conductivity decreases with reducing dimension due to enhanced phonon-boundary scattering, and tends to stabilize beyond a certain dimension. Our theoretical model (eq. 14) demonstrates stronger predictive accuracy, especially below 10 nm, by incorporating boundary scattering effects more effectively. The model aligns well with experimental values reported by Li et al. [4]. Compared to the Callaway Model [15] and Jiang's Model [12], our approach shows closer agreement with experimental trends. This highlights the capability of our formulation to address nanoscale thermal transport, consistent with layered structure heat flow theories by Cahill [18].

Figure 2 represents the thermal conductivity (κ_n) for aluminium (Al) nanowires drops with grain size. As shown, enhanced phonon scattering significantly reduces the thermal conductivity at lower dimensions. Beyond a critical grain size (~ 10 nm), the reduction trend saturates, indicating diminishing size effects. Our theoretical model (eq. 14) closely follows the experimental values reported by Chen et al. [23], and aligns well across the entire grain size spectrum. Notably, our results show improved agreement over Jiang's Model [12] and the Boltzmann Transport Equation (BTE) based model [16]. This validates the robustness and accuracy of our model for predicting nanoscale heat transport in Al nanowires, supporting classical thermophysical data provided by Touloukian et al. [26].

Figure 3 illustrates the thermal conductivity (κ_N) of gold (Au) nanowires as a function of decreasing grain size. The plot shows that as grain size decreases, κ_N reduces due to increased phonon-boundary scattering. This trend is consistent with experimental observations by Sawtelle and Reed [17], particularly for nanowires below 5 nm where the deviation becomes more pronounced. Our theoretical model (eq. 14) aligns well with these experimental results, capturing the scattering behaviour more accurately than Jiang's Model [12]. Additionally, for grain sizes below 10 nm, our model outperforms the Boltzmann Transport Equation-based approaches [18] by incorporating more realistic boundary effects. This affirms the reliability of our model [20] for predicting nanoscale heat transport behaviour in Au nanowires.

Figure 4 represents the variation in thermal conductivity (κ_N) for copper (Cu) nanowires with decreasing grain size, highlighting the impact of enhanced phonon scattering. The experimental dataset by Touloukian et al. [26] is used as a benchmark for validation. Our theoretical model (eq. 14) slightly overestimates κ_N at lower dimensions but follows the experimental trend closely. In particular, it shows better consistency across the full range of dimensions than Jiang's Model [12] and the Modified Boltzmann Transport Equation (BTE) model [14]. This agreement underscores the effectiveness of integrating thermodynamic and structural parameters as formulated in eq. (13), to capture grain boundary effects. Thus, our model reliably predicts nanoscale heat conduction behaviour in Cu nanowires.

Figure 5 represents the variation of thermal conductivity (κ_N) in indium (In) nanowires as a function of decreasing grain size. The reduction in κ_N is attributed to enhanced phonon scattering at smaller dimensions. Our computed values align closely with the experimental results provided by Touloukian et al. [26], demonstrating the robustness of our theoretical model (eq. 14). While the general trend is well depicted by all models, our formulation uniquely captures the subtle decline in thermal conductivity observed in low melting point metals like In. In contrast, the Kinetic Theory-Based Phonon Transport Model [14] and Jiang's Model [12] fail to reflect these entropy- and interaction-driven deviations. This affirms the importance of material-specific phonon interactions and entropy considerations as highlighted in Kaviany's treatment [28]. Overall, our model shows superior agreement with experimental observations over existing approaches.

Figure 6 represents the thermal conductivity (κ_N) of selenium (Se) nanowires as grain size decreases. The decline in thermal conductivity is primarily due to enhanced phonon-boundary scattering effects at the nanoscale. The predictions from our theoretical model (eq. 14) show strong agreement with the experimental values reported by Singh et al. [8]. Unlike Jiang's Model [12] and the Boltzmann Transport Equation model [14], our model successfully captures the non-linear behaviour,

particularly in the low grain size regime. The inclusion of entropy-driven scattering in our formulation is essential for matching experimental data trends more precisely. Our model's better alignment with experimental data, in contrast to the existing model by Zou and Balandin [29], confirms its validity for low-dimensional systems like Se nanowires.

Figure 7 illustrates the grain size dependent thermal conductivity (κ_N) of silicon (Si) nanowires, highlighting a distinct non-monotonic trend that contrasts sharply with the behaviour observed in metal nanowires (Figures 1–6). As the nanowire dimension (D) increases from 1 nm to 15 nm, κ_N initially drops sharply and then gradually stabilizes beyond approximately 12 nm. This reverse behaviour is primarily attributed to the semiconducting nature of silicon, where phonon transport, rather than electron transport, predominantly governs thermal conduction. Unlike metals, where increasing grain size reduces boundary scattering and enhances conductivity, silicon exhibits complex phonon dispersion relations and low group velocity modes, leading to enhanced phonon-phonon interactions at intermediate grain sizes. Consequently, intrinsic anharmonic scattering becomes dominant, causing κ_n to saturate. Moreover, quantum confinement effects in Si significantly shift phonon frequencies and Debye temperature, further influencing thermal transport. Among all models presented, including Jiang's Model [12] and the Maxwell–Boltzmann transport equation model [13], our model (Eq. 14), which incorporates entropy-driven phonon scattering and phonon frequency shifts, shows the closest agreement with experimental values reported by Chen [5]. This validates our model's robustness in capturing the complex size-dependent thermal transport phenomena in semiconductor nanowires.

4. Conclusion

This study presents a refined theoretical model (Eq. 14) to analyse the influence of grain size on thermal conductivity (κ_n) in nanomaterials by incorporating phonon scattering, vibrational entropy, and quantum confinement effects. Validated across seven materials metals (Ag, Al, Au, Cu, In), a metalloid (Se), and a semiconductor (Si), the model shows excellent alignment with experimental data, particularly below 10 nm. It effectively captures both monotonic and non-monotonic κ_n behaviour that earlier models, such as Jiang and Lu, fail to predict.

The model's strength lies in its general applicability and physical realism. It addresses structural imperfections through size-dependent scattering (γ/D^n) and entropy effects, offering predictive capability across diverse systems. Applications include: Thermoelectric materials, Nano-electronic heat management, Composite thermal design and Thermal barrier engineering.

Overall, this work advances understanding of size-dependent heat transport and offers a practical tool for material scientists and engineers in thermal management and nanotechnology.

In future studies, machine learning models [30] could be incorporated to optimize the thermal parameters such as γ and δ , and improve predictive capability across a number of new nanomaterials. The implications of incorporating temperature-dependent modelling, quantum transport frameworks, and experimental verification via TDTR and 3-Omega could further propel the applicability of the models in future nano-electronic and thermoelectric applications.

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