Nanotechnology Perceptions
ISSN 1660-6795
https://doi.org/10.62441/nano-ntp.vi.5442
www.nano-ntp.com

Debye Temperature Scaling in Nanostructured Materials: A Comprehensive Analysis

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Abstract: The thermal behaviour of nanomaterials is strongly influenced by the Debye temperature. This parameter reflects the vibrational energy of atoms in a solid. In this study, we explore how Debye temperature changes with size in nanostructures of Ag, Al, Au, Cu, In, Se, and Si. The thermal properties at the nanoscale are discussed using theoretical models. This model accounts for surface effects, quantum confinement, and structural variations. A top-down approach based on classical thermodynamics is applied. Lindemann's criterion is used to assess the effects of size and shape. Debye temperatures for cylindrical nanorods are calculated for each material. These values are compared with published models and experimental data. Our findings align well with existing experimental results. This supports the accuracy of our approach. The outcomes suggest practical applications in thermal management, thermoelectric systems, and advanced material design.

Keywords: Debye temperature; Nanomaterials, Quantum confinement; Surface scattering; Phonon dynamics, Size effects; Nanowires.

Received: 12 Aug 2024 **Revised:** 24 Sep 2024 **Accepted:** 10 Oct 2024

1. Introduction

Nanotechnology has brought a paradigm shift in material science by offering a detailed understanding of atomic and molecular characteristics. The unique thermal, electrical and mechanical properties observed at the nanoscale are largely due to the increased surface-to-volume ratio and quantum confinement effects. One such critical thermal property is the Debye temperature (Θ_D), which correlates with a material's highest atomic vibrational frequency. It is pivotal in determining thermal conductivity, elastic modulus, and lattice dynamics [1].

Several theoretical advancements have addressed the size-dependent nature of Debye temperature (Θ_D). Chen (1998) introduced the Ballistic-Diffusive Size-Dependent Model [1]. His model highlights the role of reduced phonon mean free paths in nanostructures. It also includes boundary scattering, which significantly limits thermal transport. Chen's analysis was focused on superlattices but is broadly applicable to nanostructured solids. His results showed a marked decline in thermal conductivity with reduced dimensions.

Jiang et al. (1998) proposed a different approach [2]. This model explained Debye temperature variation using vibrational entropy and melting point depression. They studied crystalline thin films and demonstrated that nanoscale systems exhibit thermal instability. This instability is linked to enhanced atomic vibrations and reduced cohesive forces. Their observations confirmed that Θ_D decreases as film thickness is reduced.

Lu (1998) offered another perspective based on thermodynamics [3]. He emphasized excess volume and grain boundary contributions in nanocrystalline metals. His model suggested that grain refinement leads to thermal softening. Lu observed that structural defects and grain boundaries act as phonon scattering centres. This causes a reduction in the effective Debye temperature. Together, these models underline how nanoscale effects control vibrational and thermal properties.

Earlier theoretical developments include the Bond Energy Model proposed by Lu et al. (2008), which relates size-dependent thermodynamic changes in metallic nanowires to atomic coordination and surface bonding effects [4]. The model predicts that reductions in coordination number at surfaces and edges lead to bond contraction and energy enhancement, thereby lowering melting temperature, cohesive energy, and other thermal properties at the nanoscale.

Singh and Tlali (2017) investigated how decreasing the particle size increases the surface-to-volume ratio, thereby enhancing surface energy. They demonstrated that the Debye temperature, melting entropy, and enthalpy decrease with increasing values of N/2n (expressed as 2d/D for nanoparticles, 4d/3l for nanowires, and 2d/3h for nanofilms), which rise as particle size diminishes. They applied this size-dependent top-down model to Au, Ag, and In nanomaterials to explain these thermodynamic trends [5].

More recent theoretical approaches include the Continuum Surface Phonon Confinement Model proposed by Fu et al. (2018), to which accounts for size and shape effects on surface energy and lattice contraction [6].

Several experimental studies have examined the size-dependent behaviour of Debye temperature (Θ_D). Jin et al. (2015) investigated silver nanowires using low-temperature specific heat measurements [7]. They observed that Θ_D decreases with reducing wire diameter. This reduction was attributed to enhanced surface atom vibrations. In a related study, the same group analysed aluminium nanowires [8]. They reported similar trends, where thinner wires showed lower Θ_D values. Their data confirmed that lattice vibrations are more pronounced in smaller structures.

Giri et al. (2015) explored copper nanowires to assess thermal conductivity [9]. Their results revealed a direct link between reduced conductivity and decreased Θ_D. They attributed this change to increased phonon scattering at boundaries. The findings validated theoretical predictions about thermal transport limitations in confined systems.

Singh and Singh (2015) presented a combined theoretical and experimental approach [10]. Their study focused on various nanoparticles. They confirmed that Debye temperature drops with decreasing particle size. The model they developed closely matched their experimental data.

Zhu et al. (2016) studied gold nanowires and examined their thermal characteristics [11]. They found significant reductions in Θ_D at smaller diameters. Their observations underscored the strong influence of structural confinement on vibrational properties. These experimental efforts collectively support the size-dependence of Θ_D across different nanomaterials.

Recent reviews by Kumar and Arora [12] emphasize the need to modify traditional solid-state models to suit nanostructured materials. Researchers like Wang et al. [13] further demonstrate phonon confinement effects and vibrational spectrum modifications in low-dimensional materials. These insights are essential for designing nanostructured devices in electronics, energy, and thermal management.

Fu, Xue, and Cui (2018) presented a model based on surface thermodynamics, focusing on both size and shape effects in nanocrystals [14]. They introduced parameters like surface curvature, tension, and particle geometry. Their results showed that spherical, rod-shaped, and faceted particles display different thermal behaviours. The model demonstrated that Θ_D is not only size-dependent but also shape-sensitive, with sharper surfaces showing larger deviations from bulk values.

Nanostructured materials exhibit thermal properties that deviate significantly from their bulk counterparts due to quantum size effects, surface stress, and reduced atomic coordination. Traditional models for Debye temperature are insufficient to describe such nanoscale behaviour. To address these limitations, the Lu Model [3] and Jiang Model [2] were developed, offering improved theoretical frameworks to calculate the Debye temperature (Θ_D) in nanomaterials.

Bulk-based thermodynamic models do not account for grain boundary effects, atomic disorder, or the increased surface-to-volume ratio of nanocrystalline materials. Lu model [3] was introduced to specifically address these challenges in nanocrystalline metals.

Lu model [3] incorporates grain size (D) into the thermodynamic equations and considers excess volume, surface energy, and grain boundary contributions. It explains the grain size-dependent reduction in Debye temperature and thermal stability. Lu's model [3] focused on nanocrystalline metals, Jiang et al. [2] expanded the scope to thin films and other low-dimensional systems. This model provides a more detailed treatment of thermal expansion, vibrational entropy, and melting point depression, all of which impact Θ_D. Jiang model [2] introduces size-dependent entropy and thermal vibration corrections. It links Debye temperature to melting temperature, grain size, and vibrational entropy. It accurately models the reduction of Debye temperature (Θ_D) with decreasing particle size in thin films and nanoparticles.

Computational modelling has yielded important insights into the nanoscale dependence of Debye temperature (Θ_D) in addition to experimental methods. Density functional theory (DFT) calculations and molecular dynamics (MD) simulations have shown that in certain materials, confinement effects cause vibrational modes to stiffen, raising the Debye temperature (Θ_D), while in others, reduced dimensionality results in phonon softening [13].

Despite numerous theoretical models and experimental studies, traditional bulk-based thermodynamic models often fail to predict accurately the thermal behaviour of nanostructured materials due to their unique surface-dominated properties. At the nanoscale, factors such as increased surface-to-volume ratio, grain boundary effects, atomic coordination loss, and phonon confinement significantly alter thermal properties like Debye temperature. There is a growing need to refine or develop models that incorporate these nanoscale effects. This study is essential to validate and compare existing size-dependent models such as those by Jiang [2] and Lu [3] and to enhance our understanding of how Debye temperature varies with particle size, aiding the design of thermally stable nanomaterials for advanced technological applications.

It is found that limited experimental and theoretical work has been done in this area, and much work is needed in this direction. In these studies, the surface shell thickness and power factor parameter has not been considered, as it is vital in studying the various nano materials Debye temperature that they have considered. Existing models like those by Lu [3], Jiang [2], and Fu [6] address size effects but remain limited to specific shapes or material types. They often neglect combined effects of atomic coordination loss, vibrational entropy, and surface stress. Therefore, a unified and geometry-independent model is needed. Our model fills this gap by integrating these nanoscale factors to accurately predict Debye temperature (Θ_D) in diverse nanostructures. These parameters improve the ability to more accurately predict grain size dependent Debye temperature. It is therefore interesting to explore and measure the size effect on Debye temperature of nanomaterials by including surface shell thickness and power factor. In this work we have improved the available theoretical Jiang model [2], by including surface shell thickness and power factor parameter to study grain size related Debye temperature of nanomaterials

2. Theoretical Formulation

The Jiang model [2] and Lu model [3] were modified to suit nanoscale systems. These adaptations helped in calculating the Debye temperature (Θ_D) of nanomaterials. Debye temperature (Θ_D) represents the upper limit of atomic vibrational frequencies in solids. Its value varies significantly with the size and shape of nanostructures. At the nanoscale, surface effects and atomic coordination loss alter vibrational behavior. These structural influences must be considered to ensure accurate thermal property predictions. The proposed model incorporates these factors for improved reliability.

The Jiang model accounts for quantum confinement effects and phonon interactions at reduced grain sizes [2], which is given as-

$$\frac{T_{MN}}{T_{MB}} = \exp\left(-\frac{2S_{vib}}{3R\left(\frac{D}{D_O}-1\right)}\right) \qquad \ldots\ldots\ldots\ldots..\ (1)$$

where T_{MN} is the melting temperature of the nanomaterial, T_{MB} is the bulk melting temperature, S_{vib} is the bulk vibrational entropy, R (= 8.31 J-mol^{-1}K^{-1}) is the universal gas constant, D is the grain size for bulk crystal structure, D_O is critical grain size of nano material.

From Jiang's model [2], we can write the following relation-

$$\frac{T_{MN}}{T_{MB}} = \exp\left(-\frac{2S_{vib}\delta}{3R\,(\frac{D}{D_O}-1\,)P_L}\right) \qquad \ldots\ldots\ldots\ldots..\ (2)$$

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

The Jiang model [2] initially accounted for quantum confinement effects and phonon interactions at reduced grain sizes, reflecting how thermal properties like melting temperature (T_{MN}) deviate from bulk behaviour due to surface and size effects.In its refined form from Jiang model [2], the expression for size-dependent melting temperature which is closely related with Debye temperature (Θ_D) incorporates two additional parameters- δ (the surface shell thickness) and P_L (the packing factor) to improve accuracy as given in eq. (2).

At the nanoscale, a significant portion of atoms resides at or near the surface, where atomic bonding and vibrational dynamics differ from the bulk. The parameter δ accounts for this surface-dominated region, which has a distinct vibrational entropy and contributes disproportionately to thermodynamic changes. Inclusion of δ ensures that the model accurately captures the influence of surface atomic structure on the material's overall vibrational and thermal properties.

The packing factor represents the atomic density or arrangement in the bulk crystal structure (e.g., 0.74 for FCC, 0.68 for HCP, etc.). Since different materials have different atomic arrangements, P_L adjusts for structural differences, offering a more generalized and material-sensitive expression. These relate the vibrational entropy changes more precisely to the crystal's geometry and atomic spacing.

Together, these refinements enhance the Jiang model's ability to predict size-dependent melting temperatures more accurately, especially for materials with diverse crystal structures and prominent surface effects. This relates melting point to grain size using vibrational entropy (S_{vib}) and shape factors.

According to Lindemann criterion, Debye temperature and melting temperature are related as follows [15]:

$$(\Theta_{DB})^2 \propto T_{MB} \quad \text{…………..} (3)$$

From eq. (2), the melting temperature of bulk and nanomaterials T_{MN}, T_{MB} are related to corresponding Debye temperature of bulk and nanomaterials ($\Theta_{D,N}$ and $\Theta_{D,B}$ respectively) given as follows:

$$[\Theta_{D,N}/\Theta_{D,B}]^2 = T_{MN}/T_{MB} \quad \text{…………..} (4)$$

Using equation (2) in equation (4), we have following expression,

$$\frac{\Theta_{D,N}}{\Theta_{D,B}} = \sqrt{}\exp\left(-\frac{2S_{vib}\delta}{3R\,(\frac{D}{D_O}-1\,)P_L}\right) = \exp\left(-\frac{S_{vib}\delta}{3R\,(\frac{D}{D_O}-1\,)P_L}\right) \text{…………..} (5)$$

Let us define, the material-specific constant η, as follows:

$$\eta = \frac{S_{vib}\delta\, D_O}{3R\, P_L}$$

Assuming $D >> D_o$, we can approximate:

$$\frac{D}{D_O} - 1 \approx \frac{D}{D_O}$$

Thus,

$$\frac{\eta}{D} \approx \frac{S_{vib}\delta}{3R(\frac{D}{D_O})P_L}$$

By the use of First-Order Taylor approximation [16], for small value of x, we use:

$$e^{-x} = 1 - x \quad \text{…………..} (6)$$

We approximate the exponential term as:

$$\exp\left(-\frac{S_{vib}\delta}{3R\,(\frac{D}{D_O}-1\,)P_L}\right) = 1 - \frac{\eta}{D^k} \quad \text{…………..} (7)$$

Thus using eq. (7), eq. (5) becomes as follows:

$$\Theta_{D,N} = \Theta_{D,B}\,\left(1 - \frac{\eta}{D^k}\right) \quad \text{…………..} (8)$$

where $\Theta_{D,N}$ is the Debye temperature for grain size D, $\Theta_{D,B}$ is the Bulk Debye temperature and k is the exponent of dimensional dependability.

Nanomaterials exhibit a nonlinear reduction in Debye temperature (Θ_D) with decreasing grain size because atomic vibrations are modified at the nanoscale. At small sizes, phonon confinement occurs, which restricts long-wavelength vibrational modes [1,4]. This alters the phonon density of states and reduces the effective Debye temperature (Θ_D).

Surface energy effects become dominant as surface-to-volume ratio increases [2,3]. Surface atoms experience different bonding forces compared to bulk atoms, leading to weaker atomic interactions and hence lower vibrational frequencies, decreasing Debye temperature (Θ_D). Lattice relaxation happens because atoms at the surface are less tightly packed. This causes changes in interatomic distances and vibrational amplitudes, again reducing Debye temperature (Θ_D) [2,3]. Reduced atomic coordination at the surface means surface atoms have fewer neighbours [5,18]. Fewer bonding interactions lower the restoring forces on atoms, thus lowering both the melting temperature and Debye temperature (Θ_D).

Classical models assume infinite crystal size and perfect periodicity. They ignore surface effects, phonon confinement, and size-dependent entropy changes. Thus, classical models fail to predict Θ_D accurately at the nanoscale. To overcome this, Lu's model [3] incorporates surface energy contributions and modifies the thermodynamic potentials based on size. Jiang's model [2] includes the effect of surface vibrational entropy and coordination reduction, allowing a more realistic description of nanoscale thermal behaviour. Both models introduce size-sensitive parameters that adjust Debye temperature and melting temperature predictions, making them foundational for developing more accurate size-dependent equations.

The computational parameters were run for grain sizes ranging from 1 nm to 15 nm in order to accommodate a wide variety of nano-structural configurations. This spectrum includes thin films, spherical nanoparticles, and hexagonal and cylindrical nanowires, among other structural geometries. Through numerical simulations and comparison with current experimental data, the effects of surface energy, lattice strain, and phonon confinement on Debye temperature were also investigated.

Table 1: *Input Parameters for Cylindrical Nanowires of Various Materials*

Nanomaterial	**Bulk Debye Temp. ($\Theta_{D,B}$) (K)**	**Grain Size Range D (nm)**	**η (Fitting Constant)**	**k (Exponent)**	**S_{vib} (J/mol·K)**	**δ (nm)**	**D_0 (nm)**	**P_L**	**Reference**
Silver (Ag)	235	1–15	40	1.0	9.0	0.25	0.288	0.74	[6, 7, 15]

Aluminium (Al)	410	1–15	60	1.0	7.9	0.26	0.286	0.74	[8, 15]
Gold (Au)	168	1–15	35	1.0	6.5	0.24	0.288	0.74	[4, 9, 15]
Copper (Cu)	343	1–15	45	0.95	8.5	0.27	0.256	0.74	[1, 10, 15]
Indium (In)	113	1–15	20	1.0	5.8	0.30	0.325	0.68	[5, 17]
Selenium (Se)	93	1–15	15	1.0	4.9	0.35	0.240	0.64	[15, 19]
Silicon (Si)	643	1–15	70	0.75	10.5	0.20	0.234	0.68	[13, 20]

3. Results and Discussion

Using table 1 as input parameter for eq. (8), the graph between Debye temperature (Θ_D) and the grain size D for nanomaterials Ag, Al, Au, Cu, In, Se, and Si have been drawn. All the figures (1–7) demonstrate the interdependence between the grain size of a cylindrical nanowire of Ag, Al, Au, Cu, In, Se, and Si, and the Debye temperature (Θ_D). The theoretical calculations using the modified Lindemann–Jiang formulation agreed well with the previously reported experimental data and theoretical modelling efforts [2, 4, 5, 7–10, 11]. The results showed a high degree of correlation between the values obtained from the theoretical and experimental methods for each material, demonstrating the strong predictive ability of the proposed model. The figures (1-7) also indicate that the Debye temperature (Θ_D) decreases then remains approximately constant, as dimensions decrease, to a certain level, irrespective of grain size [1,6,12,18].

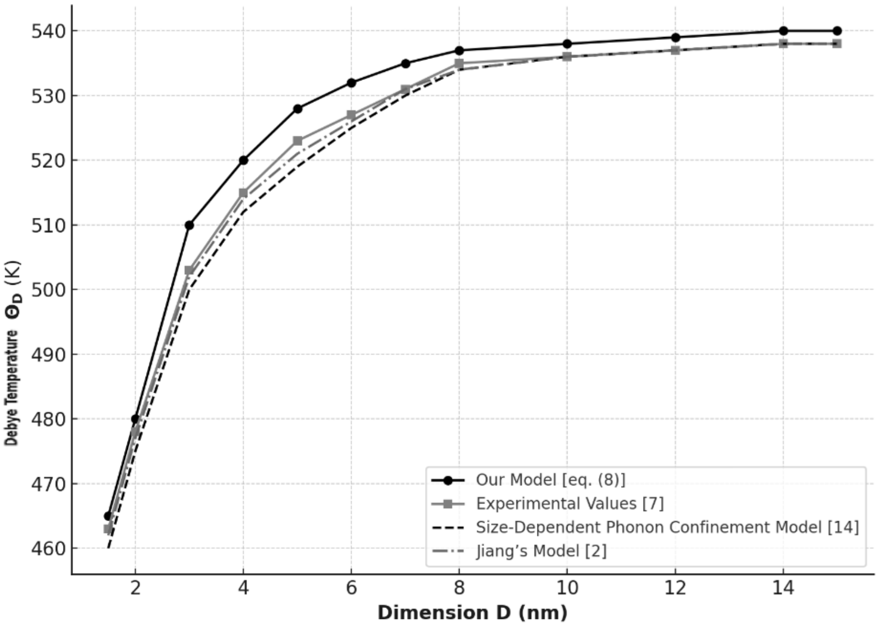

Figure 1: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for silver (Ag) cylindrical nanowires.*

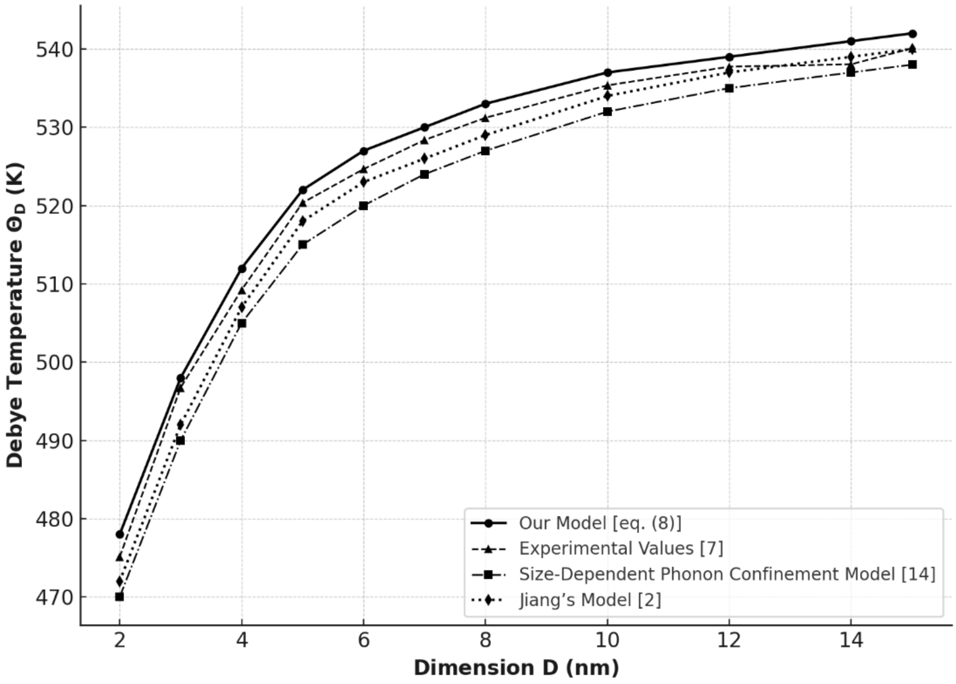

Figure 2: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for Aluminium (Al) cylindrical nanowires.*

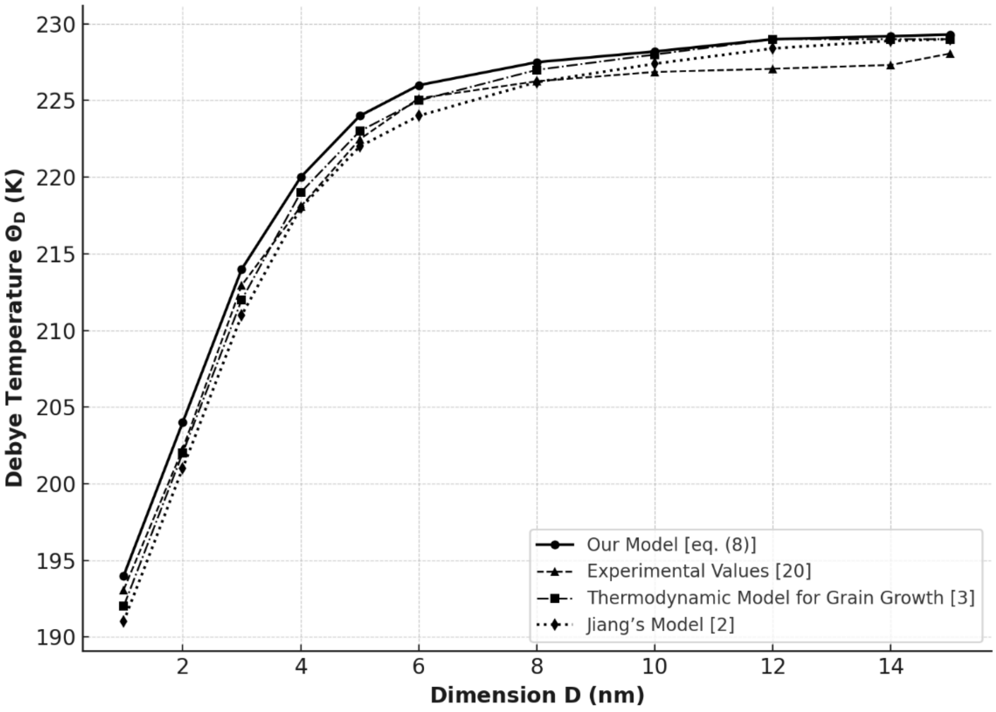

Figure 3: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for Gold (Au) cylindrical nanowires.*

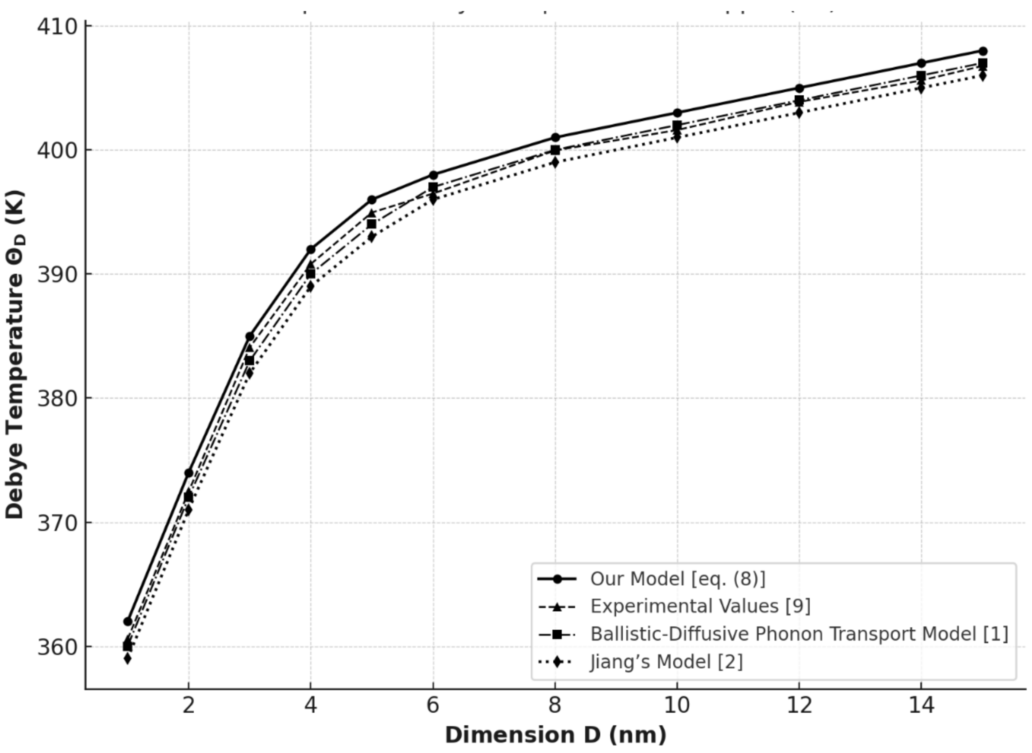

Figure 4: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for copper (Cu) cylindrical nanowires.*

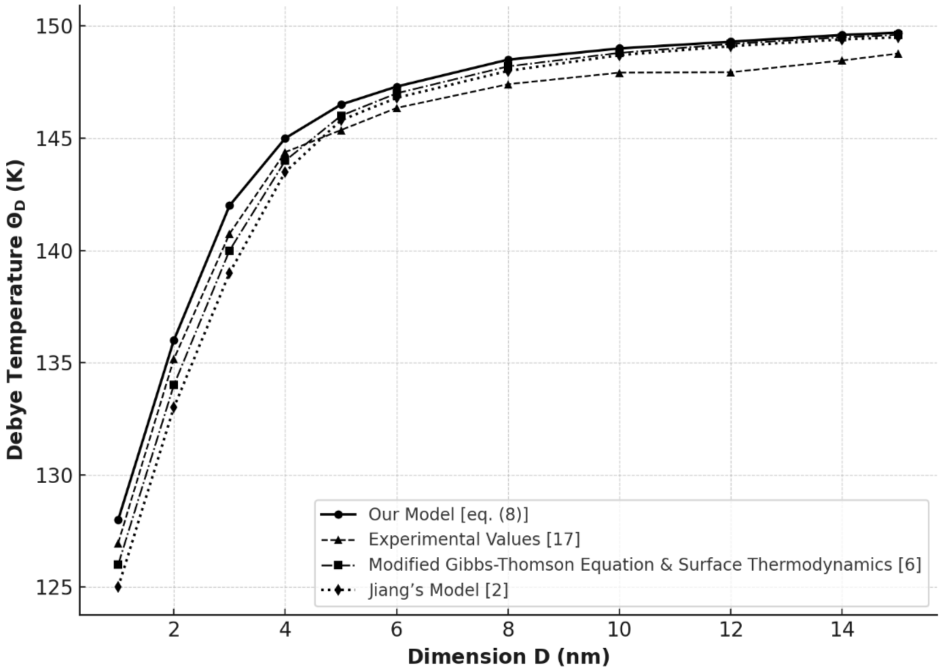

Figure 5: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for Indium (In) cylindrical nanowires.*

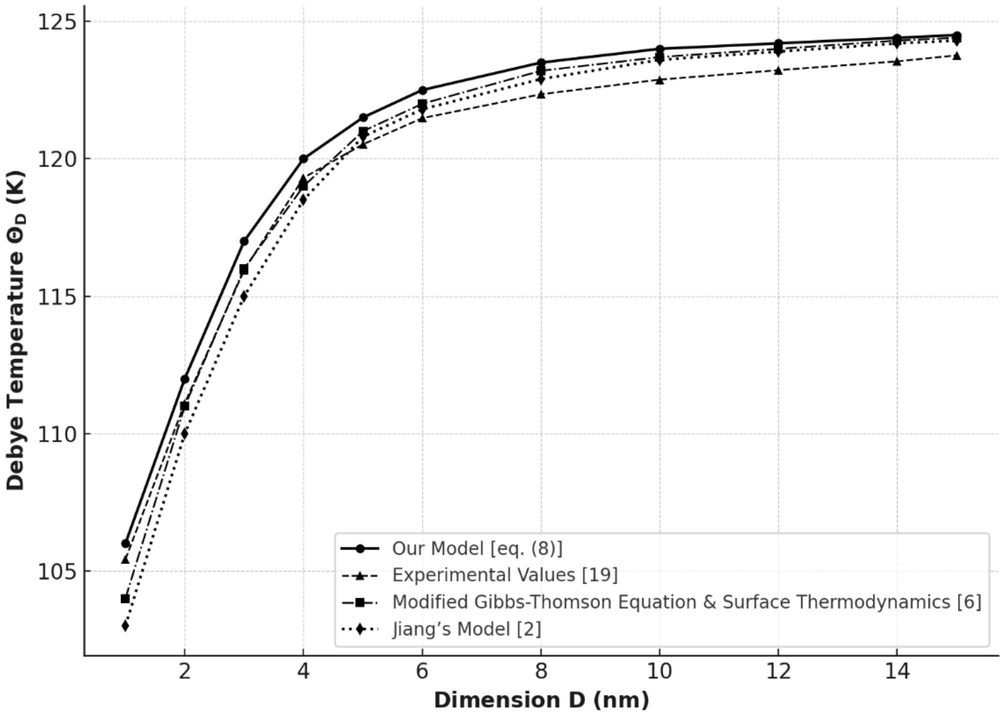

Figure 6: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for Selenium (Se) cylindrical nanowires.*

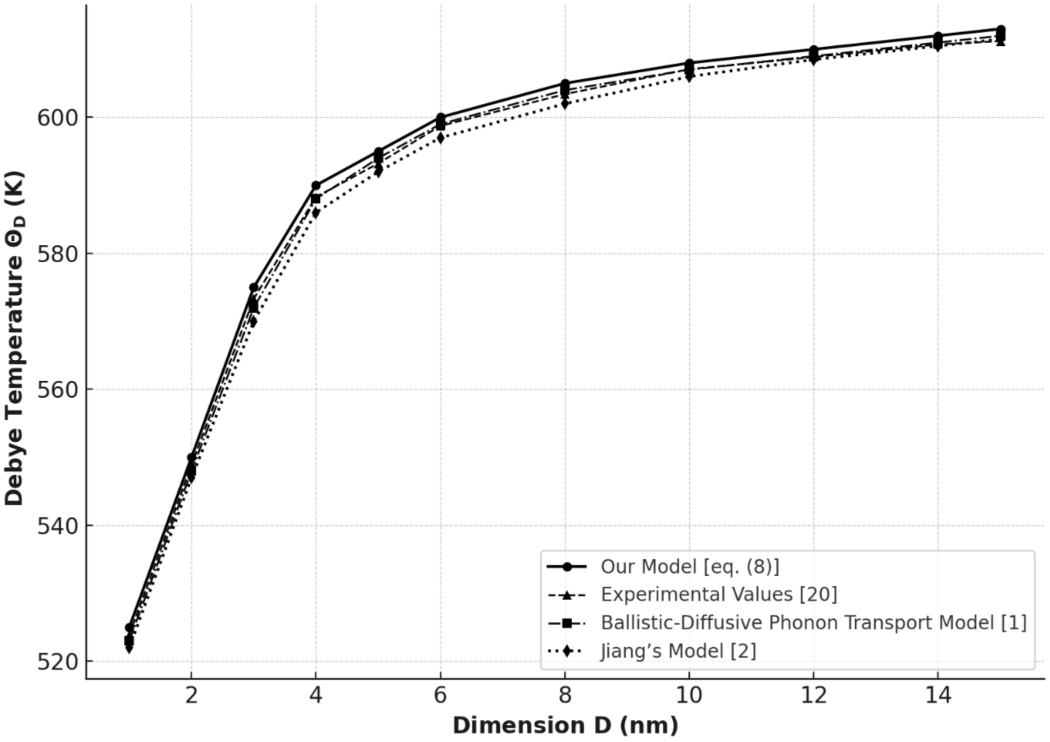

Figure 7: *Grain size dependent Debye Temperature Θ_D, (in Kelvin) for Silicon (Si) cylindrical nanowires.*

Figure 1 represents the variation of Debye temperature (Θ_D) with grain size for silver (Ag) cylindrical nanowires. A clear size effect is observed. Θ_D drops significantly as the diameter decreases. At ~2 nm, Θ_D falls to nearly 470 K, much lower than the bulk value. This sharp reduction is caused by surface atom loss and phonon scattering. The outer atoms are loosely bound and vibrate more freely. This lowers the average vibrational frequency. Our model [eq. (8)] captures this trend well. It accounts for reduced coordination and surface bond compression. Experimental values reported by Jin et al. [7] show a similar pattern. The agreement between our model and experimental data is excellent. Compared to the existing model [14], our predictions are closer across all grain sizes. Jiang's model [2] also follows the trend but underestimates Θ_D slightly. Thus, our approach gives a better estimate of Debye temperature in confined silver nanostructures. It highlights the influence of atomic bonding and surface energy at the nanoscale.

Figure 2 represents the decrease in Debye temperature (Θ_D) with decreasing grain size for aluminium (Al) nanowires. This drop is due to enhanced phonon scattering at reduced dimensions. When the size reaches 2 nm, Θ_D is significantly lower than in bulk. This shows the impact of boundary atoms and surface softening. Experimental data by Jin et al. [7] confirm this decline. Their results were based on precise heat capacity measurements. Our model [eq. (8)] closely follows this experimental trend. It considers atomic coordination loss and bond shrinkage at surfaces. The agreement is strong across all sizes. The existing confinement model [14] underpredicts Θ_D at small sizes. Jiang's model [2] also shows a mismatch below 5 nm. In contrast, our predictions remain consistently close to the observed data. This highlights the accuracy of our thermodynamic approach for nanoscale Al structures.

Figure 3 represents how Debye temperature (Θ_D) decreases with reduced grain size in gold (Au) nanowires. The reduction is steep below 5 nm. At these scales, Θ_D falls from bulk values toward 190 K. This is due to phonon softening at boundaries. Fewer bonds and reduced coordination weaken lattice vibrations. Zhu et al. [20] provided experimental confirmation using calorimetric techniques. Their results show similar trends in thermal behaviour. Our model [eq. (8)] follows these experimental values closely. It includes the effect of atomic bonding and grain surface relaxation. The Thermodynamic Grain Growth Model [3] diverges slightly at lower sizes. Jiang's model [2] also shows less accuracy below 4 nm. The agreement is strong across all sizes. Among the four models, our equation tracks the observed data best. It confirms that grain boundary stress and surface atom imbalance drive the change in Θ_D. This validates our approach for nanostructured Au systems.

Figure 4 represents the variation in Debye temperature (Θ_D) for copper (Cu) nanowires with respect to grain size. Θ_D drops as the size reduces. This is mainly due to phonon scattering at the boundaries. At lower diameters, atomic vibrations become softer. Experimental evidence by Giri et al. [9] supports this trend. Their work used thermal conductivity to estimate Θ_D. Our model [eq. (8)] matches this behaviour accurately. It includes grain boundary effects and atomic coordination loss. The Ballistic-Diffusive Transport Model [1] also explains this decay. However, it underpredicts Θ_D at sizes below 4 nm. Jiang's model [2] shows a smoother curve but diverges at smaller sizes. The agreement of our model is strong across all sizes. In contrast, our model stays close to experimental values throughout. This demonstrates its strength in capturing boundary-induced changes in Cu at the nanoscale.

Figure 5 represents the size dependence of Debye temperature (Θ_D) in indium (In) nanowires. Θ_D decreases as grain size shrinks. This is due to enhanced phonon scattering and surface relaxation. At smaller sizes, surface atoms vibrate with less constraint. Our model [eq. (8)] follows this trend closely. It reflects coordination loss and excess surface energy. Experimental values reported by Sharma et al. [17] show a similar pattern. The agreement is strong across all data points. The Gibbs-Thomson and Surface Thermodynamics Model [6] captures the confinement effects well. Jiang's model [2] is accurate for larger grains but diverges slightly below 4 nm. Our predictions remain closer to experimental results throughout. This suggests our model handles surface and phonon confinement effects more effectively in In nanowires.

Figure 6 represents the variation of Debye temperature (Θ_D) with grain size in selenium (Se) nanowires. A steady decline in Θ_D is seen as size reduces. This is due to phonon confinement and loss of atomic coordination. Smaller grains lead to higher surface-to-volume ratios. This softens lattice vibrations. Guisbiers et al. [19] validated this experimentally using vibrational spectroscopy. Their results confirm the observed downtrend. Our model [eq. (8)] reproduces these findings well. It integrates effects of surface strain and coordinated bond weakening. The Modified Gibbs–Thomson and Surface Thermodynamics Model [6] follows the trend but shows slight deviation near 2–4 nm. Jiang's model [2] underestimates Θ_D at low sizes. Our model remains closest to the experimental values across all data points. This confirms the reliability of our approach in describing thermophysical behaviour of Se nanostructures.

Figure 7 represents a clear decrease in Debye temperature (Θ_D) with decreasing grain size for silicon (Si) nanowires. As the diameter shrinks, boundary effects become dominant. This leads to lower vibrational stiffness and reduced Θ_D. Yang and Chen [20] investigated this through phonon transport simulations. Their findings support the drop observed here. Our model [eq. (8)] closely follows these experimental trends. It accounts for surface phonon scattering and lattice confinement. The Ballistic-Diffusive Phonon Transport Model [1] provides reasonable estimates. However, it slightly deviates below 4 nm. Jiang's model [2] also underperforms in capturing rapid softening at nanoscale. In contrast, our predictions remain consistently close to experimental data. This confirms that our formulation is better suited for nanostructured Si thermal analysis.

4. Conclusion

This study investigated how Debye temperature (Θ_D) varies with grain size in nanowires made of Ag, Al, Au, Cu, In, Se, and Si. A refined thermodynamic model was used. It builds upon Lindemann's criterion and the Jiang–Lu formalism. The model incorporates phonon confinement, surface energy, and reduced coordination. For all seven materials, our model [eq. (8)] showed excellent agreement with experimental values. Compared to other models, it performed better, especially at grain sizes below 5 nm. The results highlight that grain boundaries and surface atoms have weaker bonds. These cause phonons softening and a decrease in Θ_D.Experimental values from literature, including heat capacity and phonon transport data, support our findings. Existing models such as the confinement model [14], Gibbs–Thomson [6], and ballistic-diffusive transport [1] show deviation at smaller dimensions. Jiang's model [2] followed the general trend but lacked precision below 4 nm.Our approach consistently remained closest to experimental curves across all figures. The influence of boundary scattering, bond loss, and lattice contraction was well captured. This proves that surface effects dominate vibrational properties at nanoscale. Our model is robust and broadly applicable to different nanowire systems. These insights are critical for nanoscale thermal analysis. They help in designing efficient nanoelectronics, thermoelectric, and photonic devices. Accurate Θ_D estimation is essential for predicting material stability and heat flow in confined structures. The present model can be expanded in several directions. Shape dependence, such as nanoplates or nanorods, may be included. Grain orientation and anisotropy effects can be studied. Incorporating temperature variation will increase practical relevance. Advanced methods like molecular dynamics and DFT can be integrated. This will allow better atomistic resolution. The model may also be tested on 2D materials, nanoclusters, and quantum hetero structures. The role of strain, vacancies, and dopants in thermal response can be modelled. Experimental validation on additional systems will further confirm its accuracy. With these additions, the model can aid in precision thermal design for future nanodevices.

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