RP Current Trends In Applied Sciences (e-ISSN: 2583-7486)
Vol. 5, No. 2 (April – June 2026) pp. 79–88

Cite this article: P. Kumari, S. Swaraj, M. Kumar, K. Kumar, J. Mandal, Shape, size and temperature-driven nano thermodynamic evolution in $Cu_xZn_{1-x}O$ nanomaterial, *RP Cur. Tr. Appl. Sci.* **5** (2026) 79–88.

Original Research Article

Shape, size and temperature-driven nano thermodynamic evolution in $Cu_xZn_{1-x}O$ nanomaterial

Pinky Kumari, Sonal Swaraj, Mritunjay Kumar, Krishna Kumar, Jagdhar Mandal*

University Department of Physics, Tilkamanjhi Bhagalpur University, (T.M.B.U) Bhagalpur, 812007, Bihar, India
*Corresponding author, E-mail: jmandal1284@gmail.com

ARTICLE HISTORY
Received: 15 April 2026
Revised: 27 May 2026
Accepted: 27 May 2026
Published: 13 June 2026

KEYWORDS
Surface structure; Gibbs free energy; Thermal Expansivity; Reduced dimensionality.

ABSTRACT

At the nanoscale, materials no longer follow the simple thermodynamic rules that govern bulk solids. Their behaviours become strongly influenced by particle size, shape, surface structure, and temperature leading to properties that can be tuned in ways not possible in conventional materials. In this work, the shape, size and temperature-dependent nano-thermodynamic behaviour of $Cu_xZn_{1-x}O$ nanomaterials is theoretically examined. Reduced dimensionality and compositional variation modify key thermodynamic quantities such as Gibbs free energy, entropy, heat capacity, thermal expansivity and bulk modulus. Particle geometry and surface-to-volume ratio is explicitly considered and highlights deviations from their bulk behaviour as particle size decreases. The present study shows that decreasing size and non-spherical morphologies lead to increased thermodynamic instability and suppressed thermal expansion, while Cu substitution provides an additional degree of control through defect formation and lattice distortion. These results offer a clear physical picture of nano-thermodynamic evolution in $Cu_xZn_{1-x}O$ and provide useful guidance for tailoring such nanomaterials for applications in optoelectronics, gas sensing, photocatalysis and energy-related devices operating over a wide temperature range.

1. Introduction

Nanomaterials are defined as materials owning distinguishing dimensions in the range of 1–100 nm. Due to their reduced dimensions, nanomaterials exhibit properties that differ significantly from their bulk counterparts; this is primarily attributed to pronounced surface effects and quantum confinement. These materials display incredible mechanical, electrical, physical, and chemical properties [1]. Nanoscale solids can exist in various forms such as nanoparticles, nanowires and nanofilms and the progressive reduction in crystal size gives rise to distinct thermal behaviors, which play a crucial role in the development of advanced functional materials. [2]. Furthermore, the physicochemical properties of nanomaterials which depend on their size and shape make them extremely versatile for a wide range of technological applications [3]. In recent years, the size-dependence of thermal stability in nanomaterials has emerged as a significant aspect of modern technological advancements [4]. It is well established that many physical properties including plasticity, chemical reactivity, melting point, melting entropy and enthalpy, mechanical strength, and mechanisms of crystal growth are significantly influenced by the size of nanoparticles [5]. In any nanomaterial, the total number of atoms present will be a combination of surface atoms and interior atoms. As the size of the material reduces, the total number of atoms also reduces, along with a substantial increase in the surface-to-volume ratio. Due to this, the shape of the material becomes an important factor that cannot be neglected, as the shape directly influences the surface area of the material for a particular volume.

Within the themodynamical approach, Guisbiers et al. [6] reported the size and shape effect on the melting temperature and energy band gap of TiO_2 nano-structure. The size dependent valence, conduction band gap of semiconductor nanosolids has been predicted based on a model for size dependent cohesive energy [7, 8]. According to the thermodynamic theory, the melting point is a thermodynamic property [9], which may be described by the size dependence of molar Gibbs- energy [10-12]. There are some materials which are found to become harder as the size reduces and there are some which shows softness on the size reduction [13-14].

Recent progress in synthesis methods allows one to design nanoparticles of specific shapes [15-17]. These findings demonstrate that the shape is a very important factor in defining the thermodynamic properties of nanomaterials. In macro-materials, properties such as melting points, cohesive energies, surface energies, and Debye temperatures are well defined owing to their ordered atomic structure. However, in nanomaterials, changes in their atomic structure, increased surface atoms, bonding, and edge effects cause changes in these properties, which are size- and shape-dependent.

The thermodynamic model presented by Q_i and Wang is quite popular [18]. The model, which takes into consideration the cohesive energy of a nanomaterial as a combination of the energy of interior atoms and the energy of surface atoms, along with the concept of dangling bonds, has been successful in studying various thermodynamic quantities of nanomaterials, such as Gibbs free energy, entropy, heat capacity, thermal expansivity etc [19].

2. Theory of analysis

The theoretical calculations begin with the calculation of *N/n* i.e. surface area of the nanoparticle to the base volume of nanoparticle. The ratio of the number of surface atoms to that of the total atoms is more useful in finding different thermodynamic quantities, which can be given as [20].

$$\frac{N}{n}=\frac{\text{surface area of nanoparticle/surface area of an atom}}{\text{volume of nanoparticle/volume of an atom}} \tag{1}$$

Thus, *N/n* for a spherical nanosolid is

$$\frac{N}{n}=\frac{4D^2}{d^2}\left(\frac{D^3}{d^3}\right)^{-1}=\frac{4d}{D} \tag{2}$$

For different shape of nanosolids *N/n* and *N*/2*n* is evaluated which can be shown in Table 1 as follows.

Table 1: *N/n* for different nanosolids.

Nanosolids	*N/n*		*N/2n*
Spherical	4*d/D*	[21]	2*d/D*
Nanowires	*(8/3)d/l*	[21]	1.333 *d/l*
Nanofilms	*(4/3)d/h*	[21]	0.665 *d/h*
Hexahedral	4*d/D*	[23]	2*d/D*
Octahedral	(4.898)*d/a*	[23]	2.449 *d/a*
Tetrahedral	(9.797) *d/a*	[23]	4.898 *d/a*

Cohesive Energy

Cohesive energy is an essential thermodynamic property for deriving a shape and size dependent thermodynamic properties of materials. The cohesive energy of nanomaterial is the sum of the contributions of the surface atoms and the atoms in the interior.

Q_i developed an equation of known as Qi cohesive energy model and is given as [2]

The total cohesive energy (E_{total}) of the nanosolids is given as

$$E_{total}=E_0(n-N)+\frac{n}{2}E_n \tag{2}$$

where, N stands for the number of surface atoms and n denotes the total number of atoms of nanosolids and E_0 represents cohesive energy per atom of the bulk material. $(n-N)$ is the number of interior atoms in the solid. The contribution of the interior atoms to the cohesive energy of the nanomaterials is therefore, $E_0(n-N)$.

Thus, the mathematical relation for cohesive energy E_n of nanomaterial as follows:

$$E_n=\frac{AE_{total}}{n}$$

where, A =Avogardo's number. Thus, the final expression for the cohesive energy of the nanomaterial E_N is given below and E_B represents the cohesive energy of bulk nanomaterial.

$$E_N=E_B\left(1-\frac{N}{2n}\right) \tag{3}$$

Q_i and Wang proposed a model to give the cohesive energy of nanomaterials with $\frac{N}{n}=\frac{4\alpha d}{D}$ for spherical nanosolids and bulk cohesive energy per atom (E_0) is given as:

$$E_N=E_0\left(1-\frac{3N}{4n}\right) \tag{4}$$

Gibbs Free Energy (GFE)

The Debye model of Helmholtz free energy for bulk material is generalized to Gibbs free energy (GFE) model for nanomaterial, while a shape factor is introduced to characterize the shape effect on GFE.

The total Gibbs free energy [22] for spherical nanosolids in term of Helmholtz free energy per mole atom is given as Let $E=E_N N_A$ with N_A being the Avogadro constant by the elementary charge.

$$F(T,V)=E+3RT\ln\left(1-e^{\left(-\frac{\theta}{T}\right)}\right)-RTB\left(\frac{\theta}{T}\right)+\frac{4\alpha d}{D}RT\left[3B\left(\frac{\theta}{T}\right)-2.7\right] \tag{5}$$

where, E_N is the cohesive energy of the nanomaterials as described above, $R=k_B N_A$ represents the gas constant. d and D are the diameter of atoms and nanoparticles respectively, α denotes the shape factor defined as the surface area ratio between nonspherical and spherical nanoparticles in identical volume, k_B is Boltzmann constant, T is temperature, θ is the Debye temperature which is equal to the multiple of compositional bulk Debye temperature of $Cu_xZn_{1-x}O$ and the size reduction factor, $B\left(\frac{\theta}{T}\right)$ is the Debye function derived as $\frac{\theta}{T}=x$ thus $B(x)=\frac{3}{x^3}\int_0^x\frac{t^3}{e^{t-1}}dt$ [23] where $\frac{t^3}{e^{t-1}}$ is Energy contribution of phonons at a given frequency, the integral part shows the Total contribution of all phonons up to x and multiplying by $\frac{3}{x^3}$ gives a properly scaled Debye function, which determines macroscopic properties like heat capacity or bulk modulus.

Specific Heat Capacity

The specific heat capacity of nanomaterials is the amount of heat required to raise the temperature of a given quantity of a nanomaterial by one degree Celsius. Due to unique properties of nanomaterial at the nanoscale, often exhibit different thermal behaviours compared to their bulk counterparts. These differences can be attributed to factors such as increased surface area to volume ratio, quantum confinement effects, which can lead to enhanced heat capacities [28].

$$C_N=C_B\left(1-\frac{3N}{4n}\right)^{-1} \tag{6}$$

Here, C_N and C_B are specific heat capacity of nanomaterials and their corresponding bulk materials respectively.

Melting Entropy:

Melting entropy [23] of nanomaterials relates to the reform in entropy when a nanomaterial transitions from a solid to a liquid state. This reform is influenced by the size and shape of the nanomaterials due to increases surface to volume ratio and reduced cohesive energy. For nanomaterials, the decrease in melting entropy with decreasing particle size is attributed to the reduced vibrational component of overall melting entropy. Melting entropy is a critical parameter that reflects the thermodynamic reforms during the phase transition from solid to liquid, and it is significantly affected by the size and shape of the nanomaterials is given as [23]

$$S_N = S_B + \frac{3R}{2}\ln\left(1 - \frac{3N}{4n}\right) \tag{7}$$

Here, S_N and S_B are melting entropy of nanomaterials and their corresponding bulk materials respectively.

Bulk Modulus and Thermal Expansivity

The relationship between the bulk modulus (B) and the volumetric thermal expansion coefficient (ξ) provides a fundamental basis for understanding size-dependent thermomechanical behaviour in nanostructured systems. Sharma et al. [25] developed a theoretical framework to describe the variation of volume thermal expansion in nanomaterials by incorporating atomic coordination effects.

According to this model, the volume thermal expansion coefficient of a nanomaterial (ξ_N) is related to that of its bulk counterpart (ξ_B) through the expression:

$$\xi_N = \xi_B \left(1 - \frac{3N}{4n}\right)^{-1} \tag{8}$$

Here, ξ_N and ξ_B are the volume thermal expansion of nanomaterials and corresponding bulk material. This formulation reflects the influence of reduced coordination number at the nanoscale, where surface atoms exhibit altered bonding environments, leading to enhanced anharmonic lattice vibrations and consequently higher thermal expansion.

For practical applications, the above relation can be reformulated in terms of geometrical parameters by expressing the surface-to-volume atomic ratio. For nanostructures of characteristic size D, the equation becomes

$$\xi_N = \xi_B \left(1 - \frac{2d}{\eta D}\right)^{-1}$$

where, η represents the atomic packing factor and D is the Spherical Nanocrystal diameter. This expression highlights that thermal expansion is strongly size-dependent and increases as the particle size decreases.

Extending this model to anisotropic nanostructures, the geometry-specific forms Thus, expression for variation of volume thermal expansion for nanowire with nanowire diameter (L) is given as

$$\xi_N = \xi_B \left(1 - \frac{4d}{3L\eta}\right)^{-1}$$

Again, expression for variation of volume thermal expansion for nanofilm with nanofilm diameter (h) is given as:

$$\xi_N = \xi_B \left(1 - \frac{2d}{3h\eta}\right)^{-1}$$

These expressions account for the dimensional confinement and altered surface atom fraction specific to one-dimensional (nanowires) and two-dimensional (nanofilms) systems.

Furthermore, Kumar *et al.* introduced a temperature-dependent modification to the thermal expansion behavior of nanomaterials by incorporating the Anderson–Grüneisen parameter (δ_T), which quantifies the coupling between thermal expansion and elastic properties. According to this approach:

$$\frac{\xi_N}{\xi_B} = [1 - \xi_N \delta_T (T - T_0)]^{-1} \tag{9}$$

where, T is the temperature and T_0 is a reference temperature (typically room temperature). The parameter δ_T characterizes the sensitivity of thermal expansion to temperature-induced changes in bulk modulus.

By substituting the size-dependent expression of ξ_N into the above relation, a combined size- and temperature-dependent model is obtained:

$$\frac{\xi_N}{\xi_B} = \left[1 - \xi_B \left(1 - \frac{3N}{4n}\right)^{-1} \delta_T (T - T_0)\right]^{-1} \tag{10}$$

This final expression captures the coupled influence of nanoscale size effects and thermal fluctuations on volumetric thermal expansion. It demonstrates that both reduced dimensions (through $\frac{N}{2n}$) and temperature elevation (through δ_T) contribute to the deviation of thermal expansion behaviour from bulk materials.

The expression for size and shape dependence of bulk modulus for different nanomaterials is given as [27] where k = 4 is dimensionless parameter and value of $\frac{N}{2n}$ is mentioned in Table 1.

$$B_N = B_B \left(1 - \frac{3N}{4n}\right)^{k} \tag{11}$$

where B_N is the bulk modulus of the nanomaterials, and B_B bulk modulus of the bulk material.

3. Results and discussion

This paper investigates the thermoelastic parameters of $Cu_xZn_{1-x}O$ nanoparticles through the effect of size, geometry, and alloy concentration (x = 0.1-0.9) with the aid of the nanoscale EOS model. It was found that all the parameters strongly depend on the size for small sizes, attributed to surface contributions like decreased coordination and bonding strength, but tend towards the bulk value as the size increases. Size is the major contributor while geometry and alloy concentration bring in minor differences.

Table 2: Shape parameter of nanomaterials.

Shape of nanoparticle	**Shape parameter (α) [26]**
Spherical nanosolids	1
Nanofilm	0.67
Nanowire	1.33
Regular hexahedral shaped (cube)	1.24
Regular octahedral shaped	1.18
Regular tetrahedral shaped	1.49

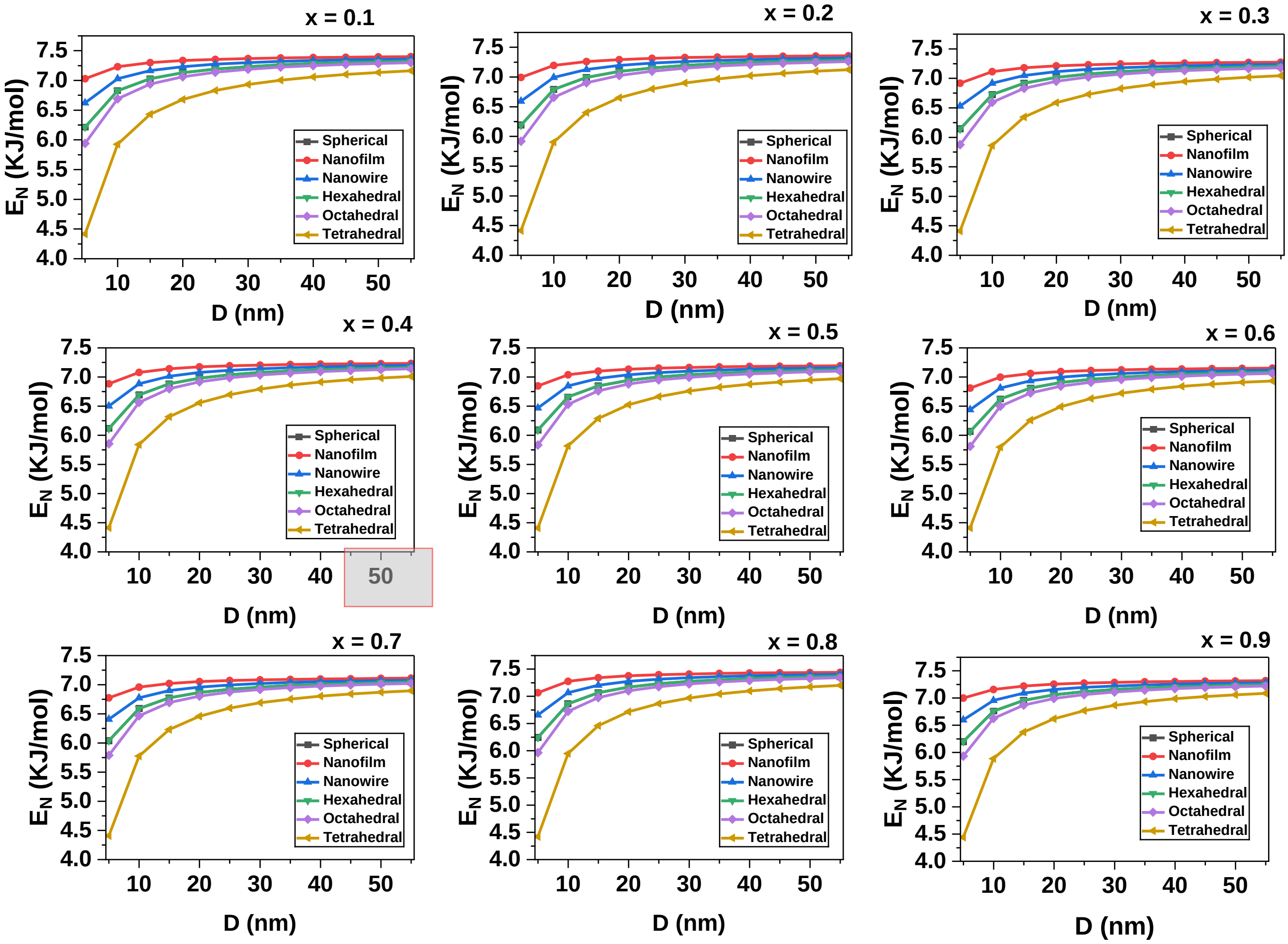

Figure 1: show the Variations of cohesive energy with the size and different geometrics for $Cu_xZn_{1-x}O$ mixed nanomaterial at concentration (x = 0.1 to 0.9).

From the results shown above, it can be observed that there is clear evidence of shape and size-dependent behavior exhibited by the $Cu_xZn_{1-x}O$ alloy nanostructure when plotted against concentrations (x = 0.1 to 0.9). For small-sized structures, all the graphs show significant fluctuations in their readings, indicating that surface atoms dominate the structure because of its high surface-to-volume ratio. This is evident from the irregular surfaces, which depict the highest deviation from the curve. Moreover, the variations seen on the graphs show the effect of shape on the property, whereby all shapes show different responses in magnitude for the property under investigation. Irregular surfaces with large contributions of surface atoms are less stable than more compact surfaces, which show greater stability. Nevertheless, at large sizes, all the curves tend to coincide, signifying that the effect of shape becomes insignificant in the bulk state.

In summary, the observations show that both the size and shape play important roles in the thermoelasticity of materials in the nanoscale regime; however, for larger sizes, the properties of the material tend to be shape-independent. This clearly favors the predictions of nanoscale EOS theories.

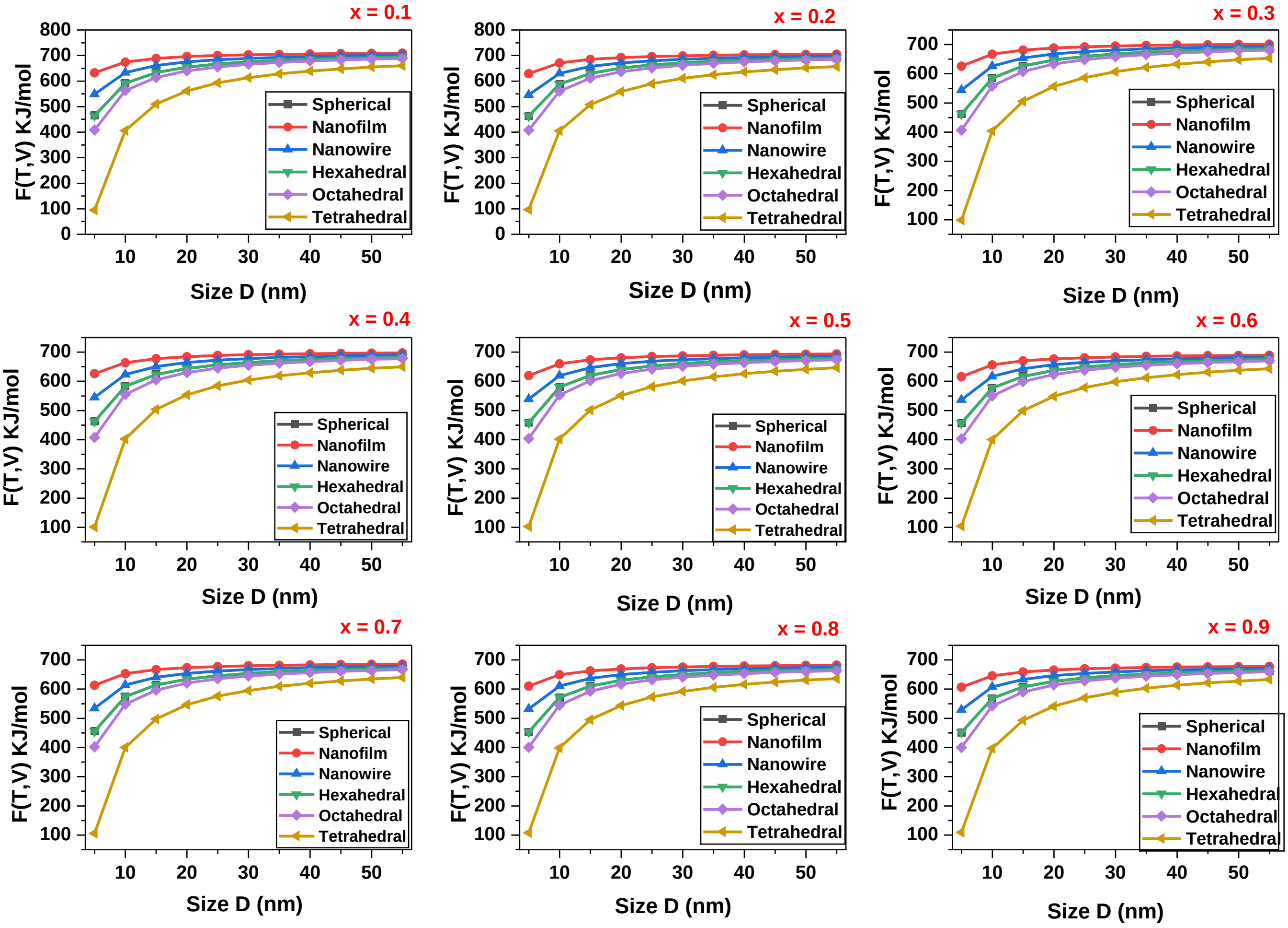

Figure 2: Shows the Variations of Gibbs Free Energy with the size and different geometrics for $Cu_xZn_{1-x}O$ mixed nanomaterial at $T = 300$ K for concentration $x = 0.1$ to 0.9.

The graphs showing Gibbs free energy versus particle size for $Cu_xZn_{1-x}O$ clearly show a size and shape-dependent trend for all compositions considered ($x = 0.1$–0.9). The values of G increase sharply with decreasing particle size and gradually stabilize at larger sizes, which implies that smaller particles are less stable compared to larger ones. This is explained by the increased role of surface atoms whose effect decreases as the particle size increases.

The difference in the behaviour between all the plotted curves corresponds to an effect due to changes in shape. The shapes with higher surface-to-volume ratios have reduced Gibbs free energy and show stronger size dependency than the rest that converge into bulk behaviour when approaching large sizes. When the composition is increased, there is a small but significant increase in Gibbs free energy, implying that there must be some change in bonding and cohesive energy as well. The effects of both composition and shape are secondary to size, though.

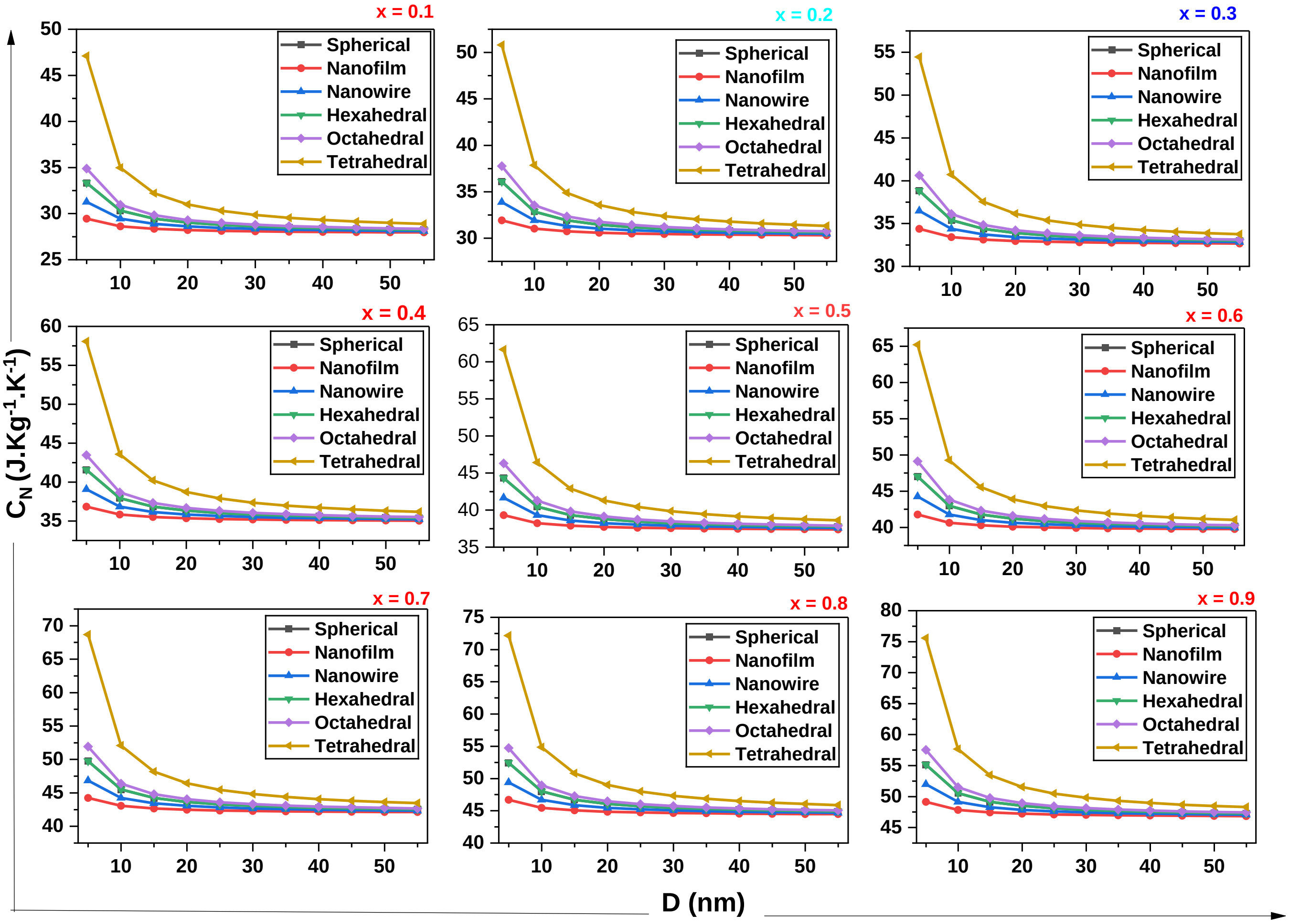

Figure 3: Shows the Variations of Specific Heat Capacity with the size and different geometrics for $Cu_xZn_{1-x}O$ mixed nanomaterial at concentration $x = 0.1$ to 0.9.

The figures given for Specific heat capacity of $Cu_xZn_{1-x}O$ represent the simultaneous effect of both shape, size and composition (x) on the thermoelastic behaviour of the $Cu_xZn_{1-x}O$ alloyed nanomaterial at concentrations $x = 0.1$ to 0.9. All the curves exhibit a steep fall at low sizes followed by a stabilization process at high sizes. The result is that at very low sizes, the properties are significantly affected by surface atoms while at high sizes, the system tends to behave in a bulk manner. It is evident from the figures that the lowest curve exhibits maximum deviation due to their relatively higher surface area while more symmetric shapes have relatively low deviation. With increased sizes, there is a tendency of merging for all the curves since size does not affect the behaviour of these systems in the bulk condition.

In addition, as the composition increases, there is a noticeable shift towards the lower side of the graph showing that composition can also influence the properties in some way but not their dependency on sizes. On the whole, the findings support the conclusion that at the nanoscale level, the behaviour of the thermoelastic properties is greatly affected by the effects of size and shape, whereas at a larger scale level, the composition effect dominates and bulk behaviour starts to prevail.

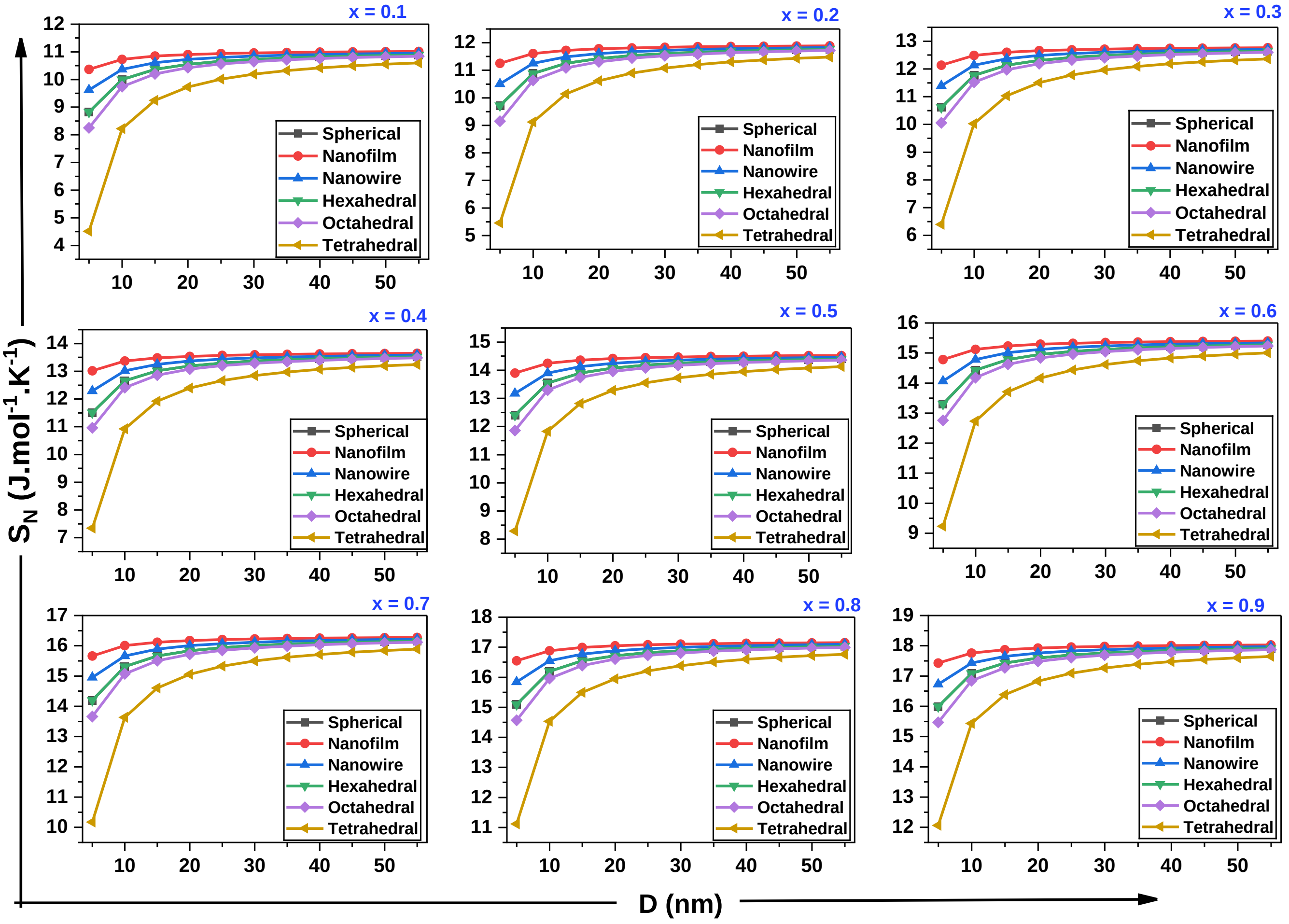

Figure 4: Shows the Variations of Melting Entropy with the size and different geometrics for $Cu_xZn_{1-x}O$ mixed nanomaterial at concentration *x* = 0.1 to 0.9.

Size dependent variation can be noticed from the graphs plotting melting entropy (S_N) versus size (D), which exist for all the compositions (*x* = 0.1-0.9). The value of S_N shows an increasing trend initially for small sizes and saturates for large sizes. This implies that there is very strong influence of surface effect on melting entropy when particle size is small and bulk effect prevails when size is high. The variation in curves is because of shape effects, wherein less compact shapes show lesser S_N than compact shapes. But all curves meet up at larger sizes, thereby confirming the fact that effects of shape become negligible in bulk limits. The value of S_N increases slightly with composition (*x*), although the nature of the plot is same. Size is thus the main factor whereas shape and composition play second fiddle.

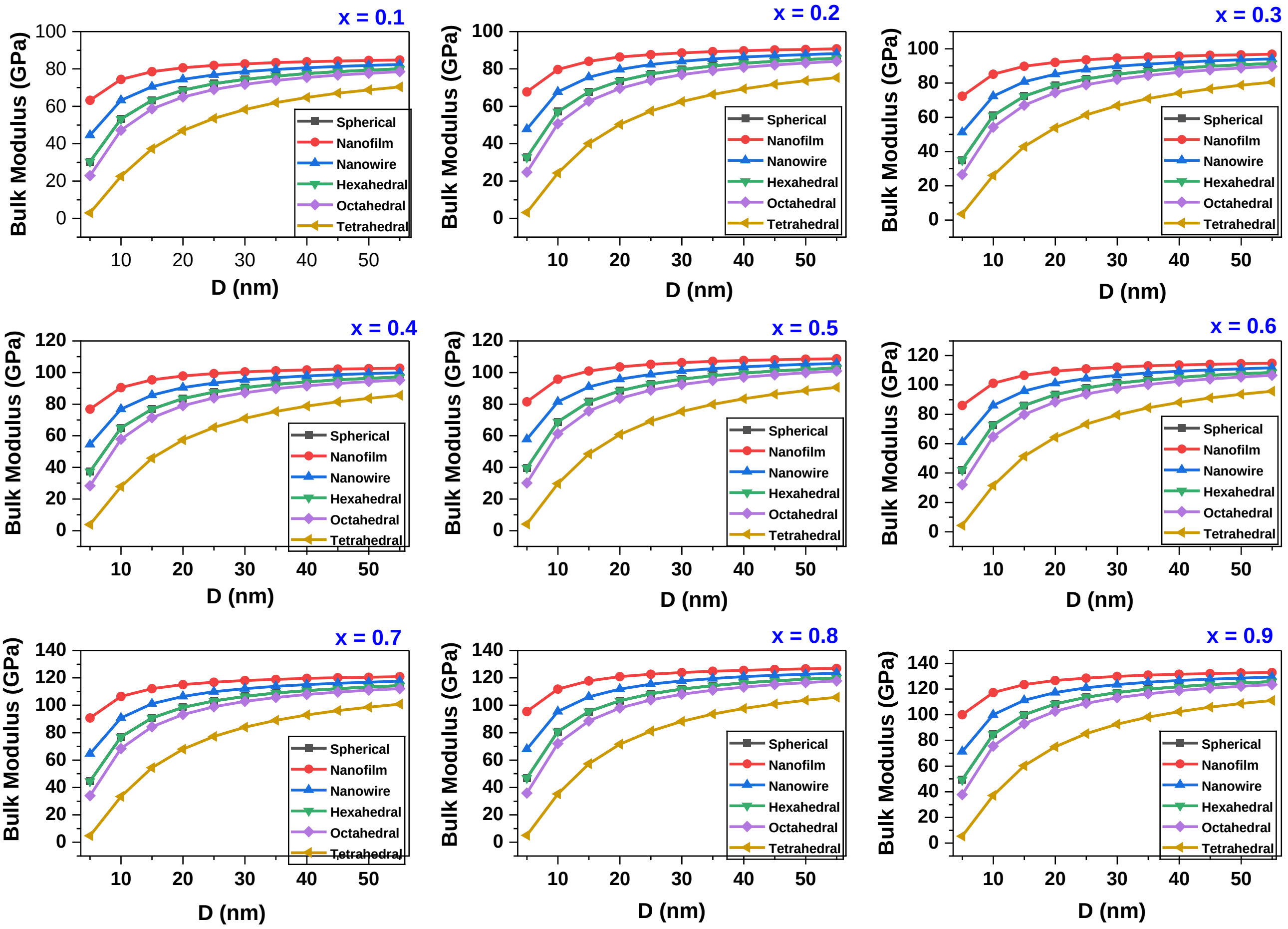

Figure 5: Shows the Variations of Bulk Modulus with the size and different geometrics for $Cu_xZn_{1-x}O$ mixed nanomaterial at concentration *x* = 0.1 to 0.9.

The plot in Fig. 6 depicts the dependence of the bulk modulus (B_N) on the particle size D(nm) of $Cu_xZn_{1-x}O$ nanomaterials for various compositions (*x* = 0.1-0.9) and geometries. For each system, there is a fast increase of bulk modulus at small sizes followed by slow convergence to a constant bulk modulus at large sizes, showing that bulk modulus grows with particle size. This is because, for nanoparticles, low coordination of the surface atoms results in decreased bulk modulus. On the contrary, an increase in the size of particles results in an increased number of bulk atoms and higher stiffness.

The dispersion of curves in the figure represents the influence of geometry, where geometries with lower compactness and higher surface-to-volume ratio display a decrease in bulk modulus compared to geometries with higher compactness. As seen, the bulk modulus increases for geometries with higher compactness. However, at large sizes, the curves intersect, which proves that the geometrical effect diminishes at large particle sizes and converges to the bulk values. A small increase in bulk modulus due to composition (x) is also evident from the curves.

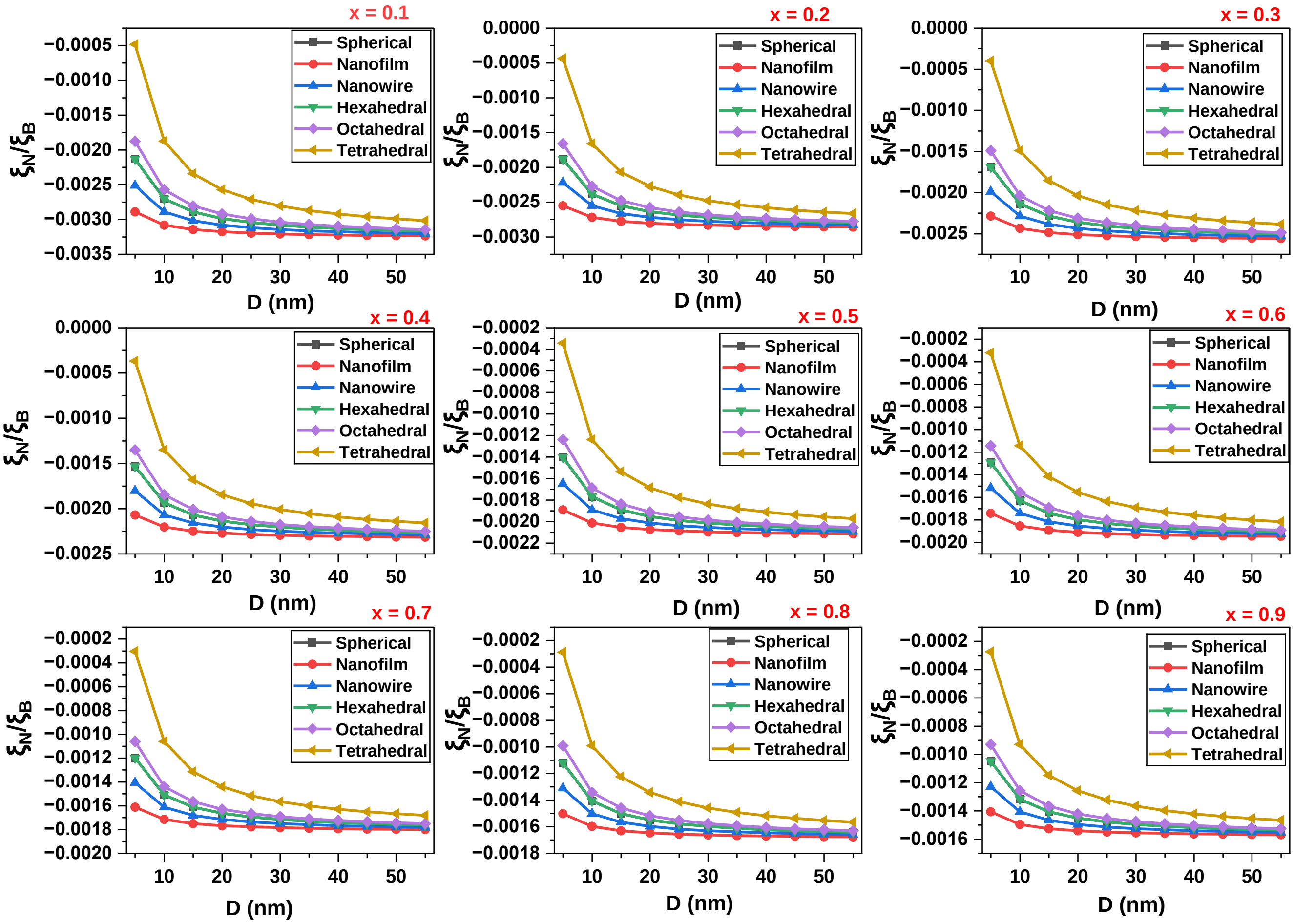

Figure 6: Shows the Variations of Thermal expansion coefficient of nanomaterials to the Thermal expansion coefficient of bulk materials $(\frac{\xi_N}{\xi_B})$ with the size and different geometrics for CuxZn1-xO mixed nanomaterial at concentration x = 0.1 to 0.9.

The variation in the normalized thermal expansion coefficient $(\frac{\xi_N}{\xi_B})$ with respect to size for different geometric shapes of $Cu_xZn_{1-x}O$ nanomaterials in the concentration range x = 0.1 to 0.9 is presented in Figure 6, which clearly demonstrates the existence of size-dependent behaviour at all concentrations. It is found that when the size is very small, the value of $(\frac{\xi_N}{\xi_B})$ is noticeably greater than one, implying that the thermal expansion of nanomaterials is significantly greater than the bulk value, whereas as the size grows, this ratio rapidly decreases initially and later on tends towards unity, which means that the system transitions from nanomaterial behaviour to bulk behavior. This pattern holds true for all concentrations because, due to the smaller coordination number of surface atoms at the nanometer scale, there is a weakening of interatomic bonding, which makes the vibrations anharmonic, resulting in increased thermal expansion. Also, the effect of geometry is important, because materials with larger surface area per volume have greater values of $(\frac{\xi_N}{\xi_B})$, whereas more dense materials have lower enhancement factors, showing the effect of geometry on thermoelastic properties. Moreover, there is a minor effect of composition, which is due to the fact that Cu and Zn atoms differ in their sizes, masses, and binding strength, resulting in changes in lattice rigidity and vibrational anharmonicity. The figure shows that thermal expansion in $Cu_xZn_{1-x}O$ nanomaterials depends mainly on the surface and size effect, along with contributions of geometry and composition, and gradually approaches bulk limit when the size grows.

4. Conclusions

In the current study, an extensive theoretical analysis of the thermo-elastic characteristics of $Cu_xZn_{1-x}O$ nano-composites has been performed by taking into account the influence of size, shape and composition. From the obtained results, it can be concluded that there is a strong correlation between the properties of interest, including cohesive energy, Gibbs free energy, specific heat capacity, melting entropy, bulk modulus and thermal expansion coefficient, and their dependency on size, especially at smaller sizes when the number of surface atoms becomes predominant due to increased surface to volume ratio. Nano-composites show substantial departure from bulk properties at extremely small sizes; however, they become closer to bulk as their sizes increase. Therefore, nanoscale thermodynamics and models used in the study are confirmed to be appropriate. Shape, quantified by shape parameter, has significant impact on deviations with more compact shapes showing better stability. Moreover, composition (x = 0.1–0.9) causes only slight differences in magnitude owing to the dissimilarity of size, mass and bonding nature of Cu and Zn atoms, but it doesn’t affect the general trend. Of all variables analyzed, the most significant controlling factor of thermo-elasticity is the size, followed by the secondary modifying parameters, namely shape and composition. In general, the research underscores that the unique features of nanomaterials result from surface effects, leading to weakening of bonds and increased anharmonicity. Also, it provides a theoretical basis for further comprehension of mixed oxide nanoparticles.

Authors' contributions

The author read and approved the final manuscript.

Conflicts of interest

The author declares no conflict of interest.

Funding

This research received no external funding.

Data availability

No new data were created.

References

[1] M. Goyal, M. Singh, Size and shape dependence of optical properties of nanostructures, *Appl. Phys. A* **126** (2020).

[2] W.H. Qi, Size effect on melting temperature of nanosolids, *Physica B: Condens. Matter* **368** (2005) 46–50.

[3] M. Ali, Modelling of size-dependent thermodynamic properties of metallic nanocrystals based on modified Gibbs-Thomson equation, *Appl. Phys. A* **127** (2021) 385.

[4] A. Gohier, C.P. Ewels, T.M. Minea, M.A. Djouadi, Carbon nanotube growth mechanism switches from tip- to base-growth with decreasing catalyst particle size, *Carbon* **46** (2008) 1331–1338.

[5] M. Singh, T.D. Phantsi, Bond theory model to study cohesive energy, thermal expansion coefficient and specific heat of nanosolids, *Chin. J. Phys.* **56** (2018) 2948–2957.

[6] G. Guisbiers, O.V. Overschelde, M. Wautelet, Theoretical investigation of size and shape effects on the melting temperature and energy bandgap of TiO_2 nanostructures, *Appl. Phys. Lett.* **92** (2008) 103121–103123.

[7] C. Yang, Q. Jiang, Size effect on the bandgap of semiconductor nanocrystals, *Solid Phenomena* **121–123** (2007) 1069–1072.

[8] M. Singh, B. Taele, M. Goyal, Modeling of size and shape dependent band gap, dielectric constant and phonon frequency of semiconductor nanosolids, *Chin. J. Phys.* **70** (2021).

[9] J. Shanker, M. Kumar, Size dependence of nanosolid properties, *Phys. Status Solidi B* **158** (1990) 11–18.

[10] G. Kaptay, Size-dependent thermodynamic properties of nanoparticles, *J. Nanosci. Nanotechnol.* **12** (2012) 2625–2633.

[11] G. Kaptay, Nanothermodynamics and size-dependent material properties, *RSC Adv.* **7** (2017) 41241–41253.

[12] P. Paneru, M. Kumar, Analysis of modified Gibbs-Thomson equation for size and shape dependence properties of nanomaterials, *High Temp.–High Pressures* **53** (2025) 507–523.

[13] G. Sharma, M. Kumar, Size and shape dependent thermodynamic properties of nanomaterials, *High Temp.–High Pressures* **44** (2015) 249–258.

[14] V. Pandey, M. Kumar, Application of size and shape dependent model for shear modulus of nanomaterials, *Indian J. Pure Appl. Phys.* **60** (2022) 951–955.

[15] A. Biswas, A. Corani, A. Kathiravan, Y. Infahsaeng, A. Yartsev, V. Sundstrom, S. De, Optical properties of nanomaterials, *Nanotechnology* **24** (2013) 195601.

[16] N. Becknell, C. Zheng, C. Chen, Y. Yu, P. Yang, Surface science studies on nanoscale materials, *Surf. Sci.* **648** (2016) 328–334.

[17] S. Zhu, C. Du, Y. Fu, Optical properties of semiconductor nanostructures, *Opt. Mater.* **31** (2009) 769–773.

[18] N. Arora, D. Joshi, Thermodynamic study of nanometals for different shapes and sizes, *Indian J. Pure Appl. Phys.* **55** (2017) 284–292.

[19] W.H. Qi, M.P. Wang, Size and shape dependent thermodynamic properties of nanomaterials, *Mater. Chem. Phys.* **88** (2004) 280–284.

[20] W. Qi, M. Wang, Q.H. Liu, Shape factor of nonspherical nanoparticles, *J. Mater. Sci.* **40** (2005) 2737–2739.

[21] W.H. Qi, Size effect on melting temperature of nanosolids, *Physica B: Condens. Matter* **368** (2005) 46–50.

[22] W. Qi, B. Huang, W. Yang, Y.J. Li, Size and shape dependent Gibbs free energy and phase stability of titanium and zirconium nanoparticles, *Mater. Chem. Phys.* **120** (2010) 446–451.

[23] S. Sharma, J. Singh, Development of size and shape dependent model for various thermodynamic properties of nanomaterials, *Physics Open* **19** (2024) 100215.

[24] C. Kittel, Introduction to Solid State Physics, 8th ed., Wiley, New York (2005).

[25] R. Kumar, G. Sharma, M. Kumar, Size and temperature effect on thermal expansion coefficient and lattice parameter of nanomaterials, *Mod. Phys. Lett. B* **27** (2013) 1350180.

[26] M. Singh, T.D. Phantsi, Bond theory model to study cohesive energy, thermal expansion coefficient and specific heat of nanosolids, *Chin. J. Phys.* **56** (2018) 2948–2957.

[27] V. Pandey, M. Kumar, Development of size and shape dependent model for bulk modulus from bulk to nanoscale, *Physica B: Condens. Matter* **629** (2022) 413617.

[28] K. Kumar, M. Kumar, S. Ahmad, A. Kumar, J. Mandal, A study of shape and size dependent thermodynamic properties of $Cu_x Al_{1-x}$ nanomaterials, *Int. J. Phys. Appl.* **7** (2025) 58–65.