

Research Article

Equations of State Based Modeling of High-Temperature Thermoelastic Properties of Selected Nanomaterials

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Abstract

Thermal expansion and temperature-dependent elastic properties are important for assessing the stability and performance of nanomaterials in high-temperature applications. The present study investigates the high-temperature thermoelastic properties of selected nanomaterials were investigated using the Murnaghan Equation of State (MEOS) and the Tait Equation of State (TEOS). The normalized volume thermal expansion, bulk modulus, and pressure–volume behavior of Fullerene, 20 nm N_i , nanocrystalline Ag, TiO_2 , Al, and Cu were evaluated over the temperature range of 300–1000 K. The ambient bulk modulus and its first pressure derivative, obtained from published literature, were used as material-specific parameters for the EOS models. The derived temperature-dependent formulation additionally employs the Anderson–Grüneisen parameter and room-temperature thermal expansion coefficient. The calculated thermal expansion results exhibit excellent agreement with theoretical predictions, demonstrating the validity of the proposed model. The bulk modulus decreases progressively with increasing temperature due to thermal expansion and the weakening of interatomic bonding, Fullerene exhibits the largest temperature-induced variation in bulk modulus, showing the highest temperature sensitivity where as Ni, Ag, TiO_2 , Al, and Cu show comparatively gradual reductions. Pressure–volume analysis reveals that pressure decreases with increasing volume expansion for all investigated nanomaterials, while TEOS predicts slightly higher tensile pressures than MEOS, particularly at larger volume expansions. Overall, both equations of state successfully describe the thermoelastic response of nanomaterials, and TEOS provides comparatively greater sensitivity for modeling high-temperature behavior. The proposed approach offers a simple, accurate, and computationally efficient method for predicting the thermodynamic and elastic properties of nanomaterials using a limited number of input parameters, making it suitable for the design of materials for high-temperature engineering and nano-device applications. The assumptions regarding temperature-independent reference parameters may, however, limit accuracy at higher temperatures.

Keywords

Temperature Dependence, Fullerene (C_{60}), Nanocrystalline Materials, Volume Thermal Expansivity, Thermoelastic Properties, Pressure–volume Relationship

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Received: 4 September 2026; **Accepted:** 16 September 2026; **Published:** 14 October 2026



1. Introduction

The Innovations in energy storage, nanomedicine, quantum devices, environmental cleanup, and sustainable technologies have been fueled by nanomaterials, which have evolved from an emerging field of study to a fundamental component of advanced scientific research in recent years. Materials with a microstructure whose characteristic length scale is on the order of a few (usually 1-100) nanometers are known as nanostructured materials (NsM) [1]. Because of their tiny size, nanomaterials are very different from bulk materials. Frequently, a nanomaterial's behavior may be more influenced by its surface area than by its actual composition. At vast scales, the electrical, optical, and chemical characteristics of nanomaterials varied greatly. Properties like reactivity, strength, electrical, and optical qualities can all be altered or improved by these parameters [2].

Fullerene (C_{60}) has garnered significant attention from the scientific community due to its exceptional structural symmetry and stability, as well as its wide range of potential uses. In recent times, nanostructures based on C_{60} have been extensively studied for various sensor technologies, such as strain sensors, gas sensors, electrochemical sensors, and optical sensors. Additionally, sensing platforms derived from fullerenes have shown a noteworthy ability to detect gases, volatile organic compounds (VOCs), metal ions, anions, and different biomolecules, underscoring their relevance in environmental monitoring, chemical analysis, and biomedical fields [3]. Nickel, a transition metal, exhibits unique catalytic and magnetic characteristics. 20-Ni has a lot of potential applications in nanostructure, including biomolecular separation, magnetic biocatalysis, pharmaceutical synthesis, and biosensors [4]. Silver nanoparticles (AgNPs) have gained considerable attention due to their unique physicochemical properties, including strong antibacterial activity, high electrical conductivity, and notable optical characteristics. These properties arise mainly from their high surface area-to-volume ratio, which enhances their interaction with biological systems. Furthermore, AgNPs can be synthesized under mild conditions (low pH, temperature, and pressure), reducing toxicity and improving biocompatibility. Owing to these advantages, AgNPs are widely explored for various biomedical and technological applications [5-7].

Titanium dioxide (TiO_2) nanomaterials are widely recognized for their unique physicochemical properties and diverse applications. They are extensively used in products ranging from sunscreens to advanced devices such as photovoltaic cells. TiO_2 nanomaterials exhibit significant potential in environmental and biomedical fields, including drug delivery, water purification, biosensing, and photocatalytic degradation of pollutants. Their high surface area, stability, and strong photocatalytic activity make them highly efficient for such applications. These advantages have driven extensive research in their synthesis, characterization, and functional optimization [8]. TiO_2 exists in three naturally

occurring crystalline polymorphs, namely anatase, rutile, and brookite. Anatase and rutile exhibit a tetragonal crystal structure, while brookite crystallizes in the orthorhombic system [9].

Thermal stability, which describes a material's ability to preserve its structural and functional properties at elevated temperatures over long service durations, has become a key focus in the development of aluminum-based nanomaterials. Enhancing this stability is essential for extending their applicability in advanced structural systems, particularly in high-performance fields such as automotive and aerospace engineering. This report presents the core principles of thermal stability in aluminum nanomaterials, including its definition, the relevant material properties, and the mechanisms of degradation under thermal and thermomechanical conditions. It also examines the effects of extreme exposures, such as accidental fire, and outlines the experimental techniques used to evaluate thermal stability [10].

Because of their improved electrical conductivity at the nanoscale, copper-based nanomaterials are appropriate for use in conductive inks and electronic devices. Effective electron transport and enhanced performance in flexible electronics are made possible by their high surface-to-volume ratio. Additionally, they have great catalytic activity and good thermal conductivity, which help energy storage and heat management applications. Their tunable optical characteristics also increase their application in photonic and optoelectronic devices [11].

In the present study, a simple theoretical framework has been developed to examine the thermal expansion behavior and bulk modulus of various nanomaterials. The Murnaghan and Tait equations of state (EOS) are utilized to evaluate the variation of relative volume (V/V_0) under elevated temperature conditions. Moreover, the obtained results are compared with alternative approaches to assess the suitability and effectiveness of these EOS in describing the temperature-induced thermal volume expansion of nanomaterials. The suggested EOS formulation is not meant to be universally applicable to all nanomaterials; rather, it is meant to serve as a generic phenomenological technique for characterizing temperature-dependent thermoelastic behavior. The correctness of the predicted thermoelastic behavior over the studied temperature range and material-specific characteristics determine how applicable these EOS are.

2. Materials and Methods

In general, materials undergo thermal expansion with increasing temperature and contraction with decreasing temperature. Within a defined temperature range, these dimensional variations are often approximated as linearly dependent on

temperature. The coefficient of thermal expansion (α) represents the proportionality factor describing this response and is a characteristic property specific to each material.

It is defined as

$$\alpha = \frac{1}{V} \left(\frac{dV}{dT} \right)_P \quad (1)$$

where V is the volume, and T the temperature.

The author [12] used the temperature dependence of α as given below:

$$\alpha = a + bT + cT^2 \quad (2)$$

Here, a , b and c are constants. It should be pointed out that Eq. (2) is not consistent with the initial boundary condition, viz.

$\alpha = \alpha_0$ at $T = T_0$. Higher-order polynomial terms, however, may make fitting more difficult and result in overfitting or unrealistic behavior outside of the temperature range under study;

In order to satisfy this condition, we write Eq. (2) as follows:

$$\alpha = a + b(T - T_0) + c(T - T_0)^2$$

or

$$\alpha = \alpha_0 + \alpha'_0 (T - T_0) + \alpha''_0 (T - T_0)^2 \quad (3)$$

where α'_0 and α''_0 are the first and second-order derivatives of α with T

It is possible to define α'_0 and α''_0 in terms of α_0 , which reads as follows [13]

$$\alpha'_0 = \alpha_0^2 \delta_T$$

$$\alpha''_0 = \alpha_0^3 \delta_T^2$$

where δ_T is called the Anderson–Grüneisen parameter.

Thus, Eq. (3) may be rewritten as follows:

$$\alpha = \alpha_0 + \alpha_0^2 \delta_T (T - T_0) + \alpha_0^3 \delta_T^2 (T - T_0)^2 \quad (4)$$

Equation (4) is true provided that α depends on T quadratically. Moreover, considering the temperature-dependence of α given by Eq. (4) neglects the higher-order terms, which may introduce the error on the temperature-dependence of α . Higher-order polynomial terms, make fitting more difficult and result in overfitting or unrealistic behavior outside of the temperature range under study; It is therefore necessary to consider the complete form of Eq. (4), which reads as follows:

$$\alpha = \alpha_0 + \alpha_0^2 \delta_T (T - T_0) + \alpha_0^3 \delta_T^2 (T - T_0)^2 + \dots \quad (5)$$

or

$$\frac{\alpha}{\alpha_0} = (1 - \alpha_0 \delta_T (T - T_0))^{-1} \quad (6)$$

Using the definition of α , the integration of Eq. (6) gives the following relation:

$$\frac{V}{V_0} = (1 - \alpha_0 \delta_T (T - T_0))^{-1/\delta_T} \quad (7)$$

Author [14] uses $\delta_T = B'_0$

where B'_0 is derivative of bulk modulus at zero temperature

The following expression for temperature dependence of $\frac{V}{V_0}$ has been obtained by Fang [15] as.

$$\frac{V}{V_0} = 1 - (\delta_T)^{-1} \ln[1 - \alpha_0 \delta_T (T - T_0)] \quad (8)$$

Assuming the fact that product of thermal expansion coefficient α and isothermal bulk modulus is constant under the effect of pressure [16]

$$\alpha B_T = \text{Constant} \quad (9)$$

On differentiating r. t. volume

$$\alpha \left(\frac{dB}{dV} \right)_T + B \left(\frac{d\alpha}{dV} \right)_T = 0$$

The Anderson -Grüneisen parameter at constant temperature

$$\delta_T = \frac{V}{\alpha} \left(\frac{d\alpha}{dV} \right)_T = - \frac{V}{B} \left(\frac{dB}{dV} \right)_T \quad (10)$$

Assuming δ_T to be independent on V

$$\delta_T = \left(\frac{dB}{dP} \right)_T = B'_0$$

Anderson-Grüneisen parameter δ_T and $\eta = \frac{V}{V_0}$ are related by the relation [17].

$$\frac{\delta_T + 1}{\eta} = A$$

Where A is constant for given solid.

Using (11) eq. (10) can be written as

$$\frac{dB}{B} = \left[-\frac{A}{V_0} + \frac{1}{V} \right] dV$$

Integrating

$$\frac{B}{B_0} = \frac{V}{V_0} \exp A \left[1 - \frac{V}{V_0} \right]$$

On expanding

$$\frac{B}{B_0} = \frac{V}{V_0} \left(1 + A \left(1 - \frac{V}{V_0} \right) + \frac{A^2}{2} \left(1 - \frac{V}{V_0} \right)^2 + \dots \infty \right)$$

Neglecting the higher order terms

$$\frac{B}{B_0} = \frac{V}{V_0} \left(1 + A \left(1 - \frac{V}{V_0} \right) \right) \quad (12)$$

Constant A is determined by initial conditions

$$\text{At } V = V_0 \frac{\delta_T^0 + 1}{1} = A$$

$$\text{Or } \delta_T^0 = B_0'$$

So eq. (12) becomes

$$\frac{B}{B_0} = \frac{V}{V_0} \left(1 + (1 + B_0') \left(1 - \frac{V}{V_0} \right) \right) \quad (13)$$

This equation can be used to study the variation of Bulk

modulus with various compression of different nanomaterials.

Other equation of states (EOS) that we include for compression purpose of nanomaterials Murnaghan equation of state (MEOS) & Tait equation of state (TEOS).

The Murnaghan equation of state (MEOS) reads as follows [26].

$$P = \frac{B_0}{B_0'} \left[\left(\frac{V_0}{V} \right)^{-B_0'} - 1 \right] \quad (14)$$

The Tait equation of state (TEOS) reads as [25]

$$P = \frac{B_0}{A} \left[\exp A \left(1 - \frac{V}{V_0} \right) - 1 \right]$$

$$P = \frac{B_0}{(1+B_0')} \left[\exp(1 + B_0') \left(1 - \frac{V}{V_0} \right) - 1 \right] \quad (15)$$

These EOS are used to study the pressure with high compression on nanomaterials.

3. Results & Discussion

3.1. Input Parameters and statistical Comparison of Investigated Nanomaterials

Table 1. Input parameters at zero pressure and room temperature of the selected nanomaterials used in the present calculations.

Materials	$\alpha_0 \ 10^{-6} K^{-1}$	$B_0 (Pa)$	$B_0' = \delta_T$	$T_0 (K)$
Fullerene C ₆₀	17.27 [18]	491 [19]	122 [20]	300
20-nm Ni	33 [21]	228 [21]	26.34 [21]	300
nm-Ag	18 [22]	103.6 [23]	4 [23]	300
nm-TiO ₂	15.2 [20]	243 [24]	4 [24]	300
nm-Al	78 [25]	321 [25]	4 [25]	300
Cu	6.2 [22]	137.8 [23]	4 [23]	300

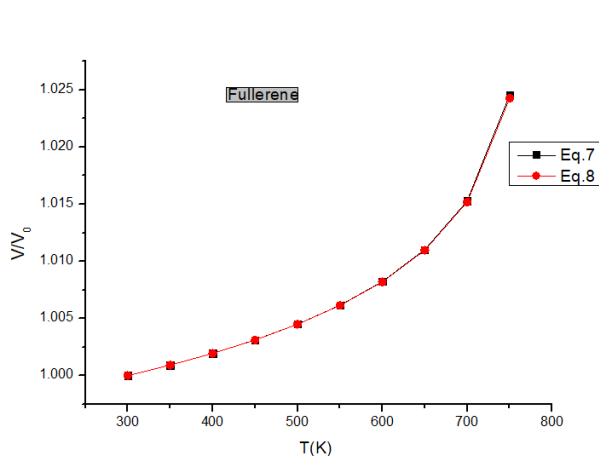
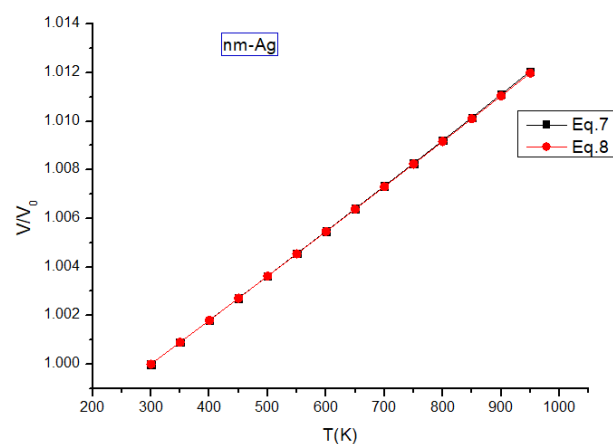
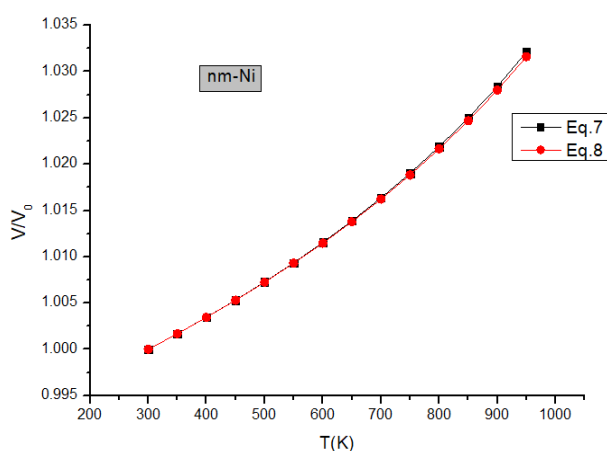
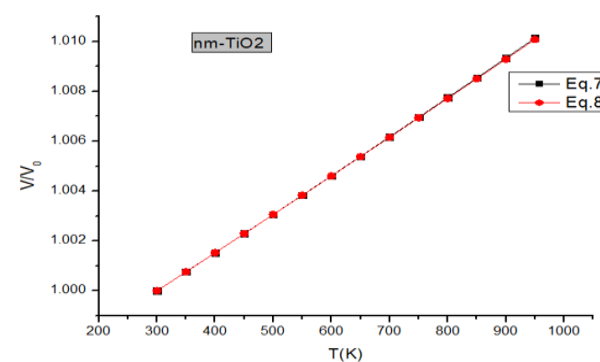
Table 2. Quantitative statistical comparison between the present and theoretical results for the investigated nanomaterials.

Materials	RMSE	MAE	Percentage error	R^2
Fullerene C ₆₀	0.0001033	0.0000542	0.00532%	0.999792
20-nm Ni	0.0002115	0.0001432	0.01399 %	0.999524
nm-Ag	0.00003379	0.00002450	0.002427 %	0.999918
nm-TiO ₂	0.00002393	0.00001750	0.001736 %	0.999942
nm-Al	0.00074706	0.00053550	0.05131 %	0.998189
Cu	0.00000391	0.00000286	0.0002848 %	0.999990

Table 3. Mean Relative deviation between TEOS and MEOS pressures at representative volume expansion ratios for the investigated nano-materials. s.

Materials	Volume change	MEOS (ΔP)(GPa)	TEOS (ΔP)(GPa)	Mean relative deviation
Fullerene C ₆₀	1.00-1.02455	0-3.82	0-4.78	25.74 %
20-nm Ni	1.00-1.03211	0-4.89	0-5.64	15.61 %
nm-Ag	1.00-1.01206	0-1.21	0-1.57	29.94 %
nm-TiO ₂	1.00-1.01013	0-2.40	0-3.05	27.36 %
nm-Al	1.00-1.0583	0-16.27	0-20.54	26.46 %
Cu	1.000-1.00407	0-0.56	0-0.71	28.77 %

3.2. Thermoelastic and Pressure–Volume Properties of Investigated Nanomaterials

**Figure 1.** Variation of volume with effect of high temperature in Fullerene (C₆₀) nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).**Figure 3.** Variation of volume with effect of high temperature in nm-Ag nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).**Figure 2.** Variation of volume with effect of high temperature in 20nm-Ni nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).**Figure 4.** Variation of volume with effect of high temperature in nm-TiO₂ nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).

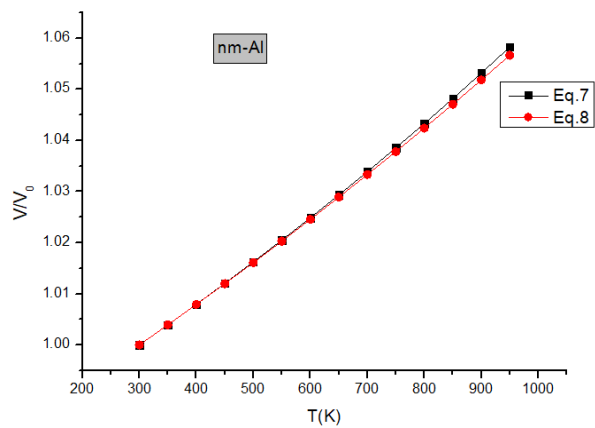


Figure 5. Variation of volume with effect of high temperature in nm-Al nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).

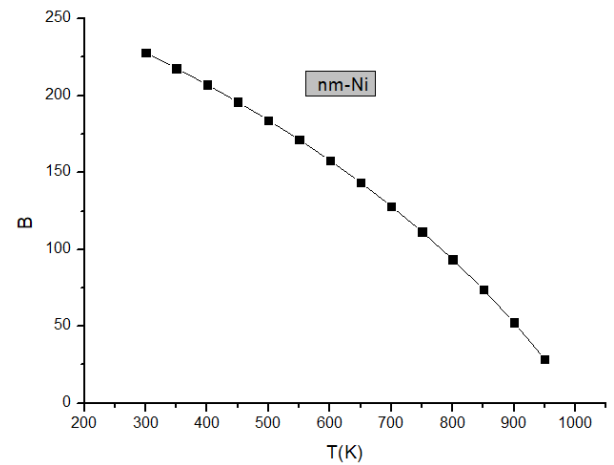


Figure 8. Variation of bulk modulus with effect of high temperature in 20nm-Ni nanomaterial with present Eq. (13).

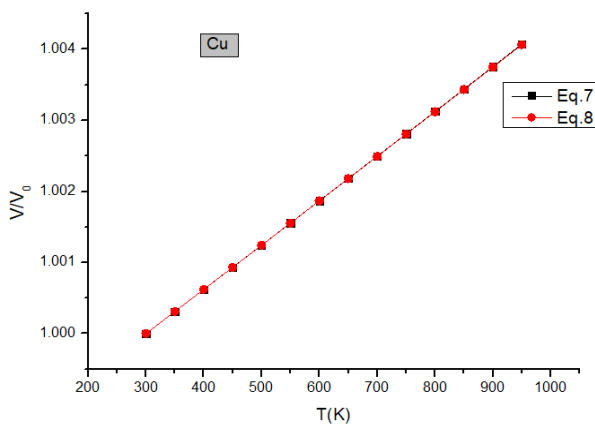


Figure 6. Variation of volume with effect of high temperature in nm-Cu nanomaterial with present (Eq. (7)) and Fang et al. (Eq. (8)).

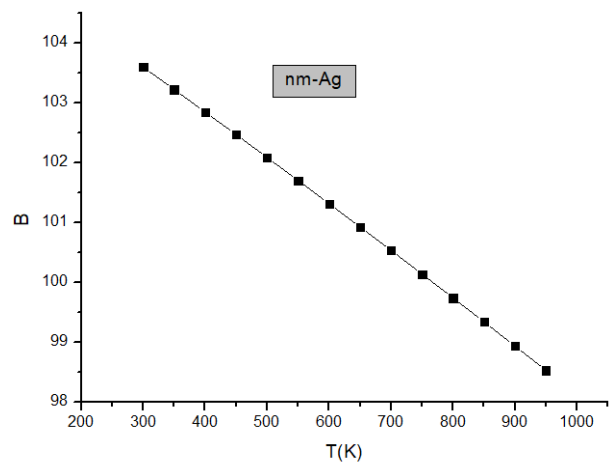


Figure 9. Variation of bulk modulus with effect of high temperature in nm-Ag nanomaterial with present Eq. (13).

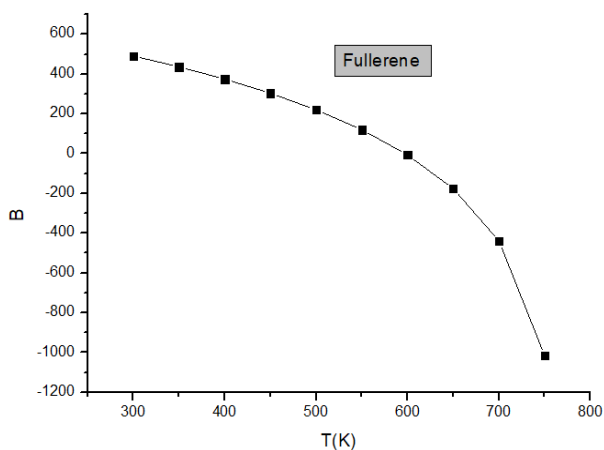


Figure 7. Variation of bulk modulus with effect of high temperature in Fullerene (C60) nanomaterial with present Eq. (13).

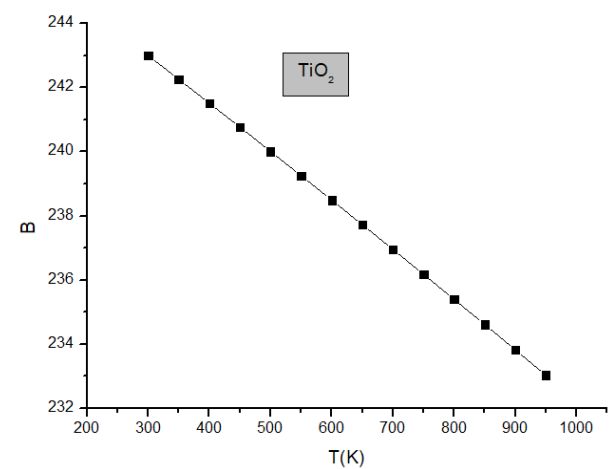


Figure 10. Variation of bulk modulus with effect of high temperature in nm-TiO₂ nanomaterial with present Eq. (13).

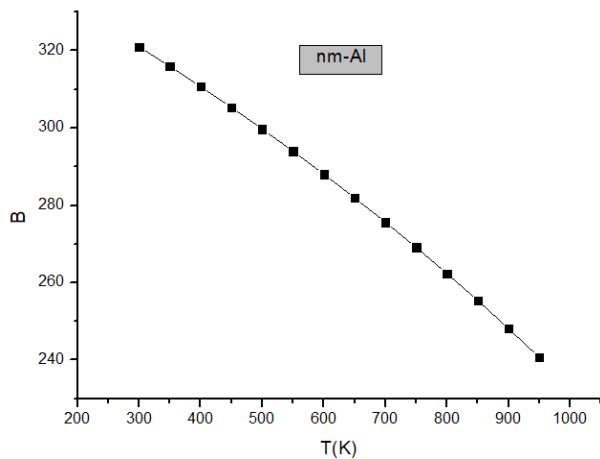


Figure 11. Variation of bulk modulus with effect of high temperature in nm-Al nanomaterial with present Eq. (13).

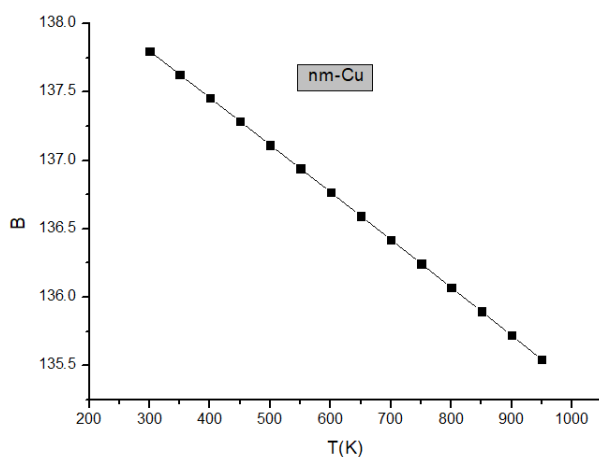


Figure 12. Variation of bulk modulus with effect of high temperature in nm-Cu nanomaterial with present Eq. (13).

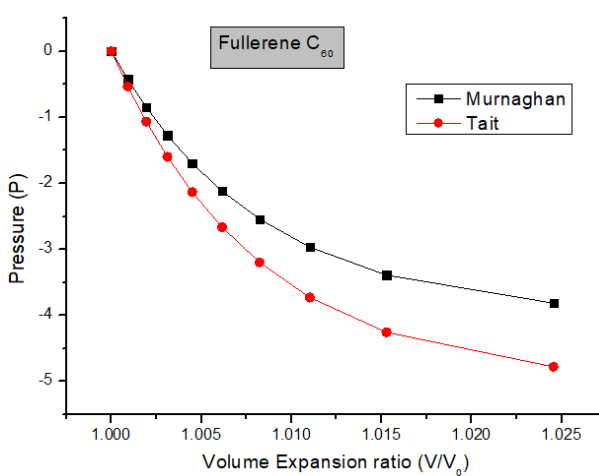


Figure 13. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in Fullerene (C₆₀) nanomaterial.

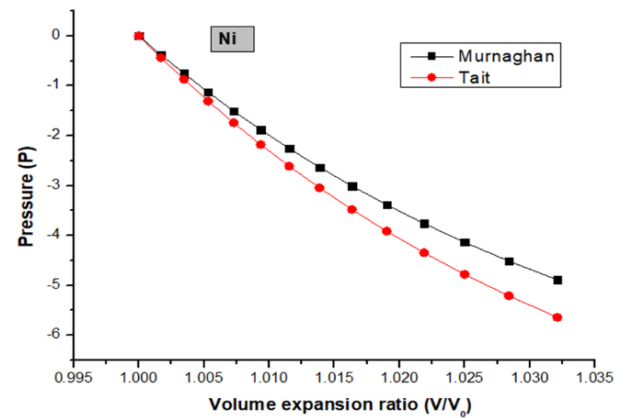


Figure 14. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in nm-Ni nanomaterial.

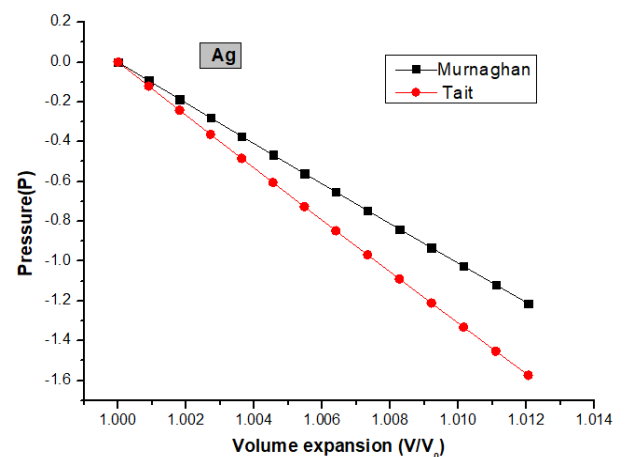


Figure 15. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in nm-Ag nanomaterial.

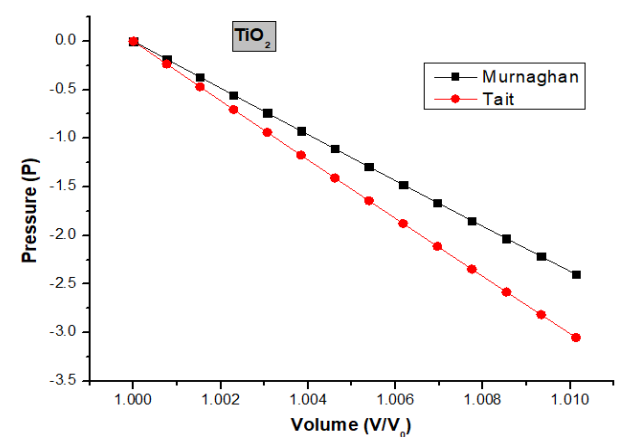


Figure 16. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in nm-TiO₂ nanomaterial.

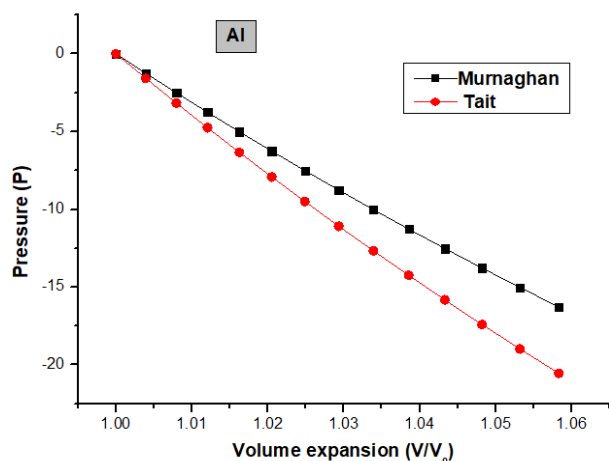


Figure 17. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in nm-Al nanomaterial.

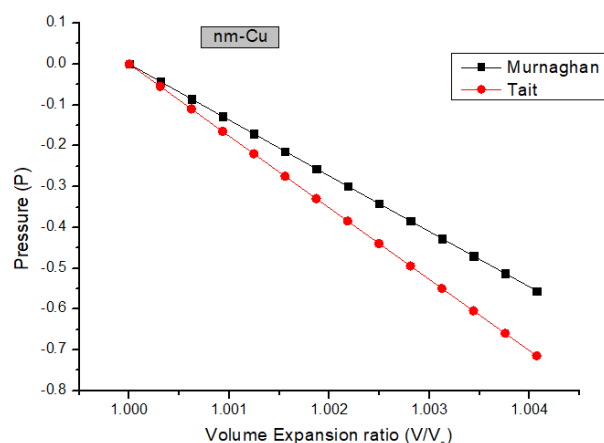


Figure 18. Comparative Variation of pressure with respect to volume expansion ratio in Murnaghan and Tait EOS in nm-Cu nanomaterial.

The Murnaghan equation of state (MEOS) and the Tait equation of state (TEOS) are two equations of state that were used in this work to examine the thermal expansion behavior of particular nanomaterials. The bulk modulus under ambient circumstances (B_0) and its first pressure derivative (B'_0) are the only two material-specific characteristics needed for both EOS models. These values were obtained from the published literature and are shown in Table 1. Derived equation (7) used to calculate the normalized volume thermal expansion ($\frac{V}{V_0}$) over the temperature range of approximately 300–1000 K. The Anderson–Grüneisen parameter (δ_T) and the room-temperature volume thermal expansion coefficient (α_0), which are both described in Table 1, are the only two input parameters needed for the suggested model. Six representative nanomaterials were calculated: Fullerene (C_{60}), 20 nm Ni, nanocrystalline Ag, TiO_2 , Al, and Cu. The computed thermal-expansion and pressure-volume curves were used to evaluate the applicability of MEOS and TEOS over 300–1000 K. Over the

tested range, both EOS show consistent and physically plausible patterns; nevertheless, their assumptions may limit accuracy at higher temperatures and bigger expansions.

Figures 1 to Figure 6 shows the temperature dependence of the normalized volume expansion ($\frac{V}{V_0}$) for various nanomaterials as determined by derived equation (7). The matching theoretical curves were compared with the computed findings. The normalized volume consistently rises with temperature in every instance, indicating the anticipated thermal expansion behavior of the nanomaterials under investigation. Over the whole temperature range taken into consideration, there is great agreement between the current estimates and the theoretical predictions. Quantitative statistical metrics, including RMSE, MAE, mean percentage error, and R^2 have been calculated for each investigated nanomaterials to quantitatively assess the agreement between the present and theoretical results. The obtained values are presented in Table 2. The suggested method for forecasting the thermal expansion behavior of nanomaterials is valid and reliable, as evidenced by the strong agreement between the two sets of findings. Additionally, the current results' agreement with the theoretical model presented by Fang et al. [15] suggests that Equation (7) offers a precise and effective description of volume thermal expansion with a small number of input parameters and allowing for the simultaneous assessment of specific nanomaterials' bulk modulus, volume expansion, and pressure-volume behavior at elevated temperatures. Therefore, compared to the volume-expansion approach described by Fang et al., the current study offers a more comprehensive thermoelastic assessment. As a result, the suggested formulation can be regarded as a straightforward and trustworthy model for assessing the thermal expansion properties of a variety of nanomaterials. Overall, the calculated results demonstrate that although all nanomaterials expand with increasing temperature, the magnitude of expansion strongly depends on their intrinsic thermoelastic properties, particularly the bulk modulus and bonding characteristics. Materials possessing lower effective stiffness exhibit larger thermal expansion, whereas materials with higher bulk modulus undergo comparatively smaller volume changes. These observations confirm that the selected equations of state successfully reproduce the expected thermoelastic response of different classes of nanomaterials.

In this paper we have also reported the result obtained for thermodynamical properties of some nanomaterials Fullerene (C_{60}), 20 nm Ni, nanocrystalline Ag, TiO_2 , Al, and Cu under the effect of high temperature. The values of input parameters are used to calculate the bulk modulus by used eq. (13) and calculated results for all nanomaterials have been shown in graphical form to show the validity of equation with available experimental/theoretical data.

The calculated results show that the bulk modulus of all investigated nanomaterials decreases with increasing temperature due to thermal expansion and weakening of interatomic forces. Fullerene (C_{60}) exhibits the highest temperature sensitivity, whereas Ag, TiO_2 , Al, and Cu show nearly linear and

gradual reductions in bulk modulus. The average temperature sensitivity of the bulk modulus is calculated as $S_B = \left| \frac{\Delta B}{\Delta T} \right|$, in order to quantify the temperature sensitivity seen in the bulk-modulus-versus-temperature graphs. Among the nanomaterials under investigation, Fullerene had the greatest temperature-induced variation in bulk modulus, according to the research. The finding that Fullerene has the highest temperature sensitivity and that the other nanomaterials exhibit relatively lower fluctuations over the same temperature range is quantitatively supported by this.

The study confirms that temperature has a significant effect on the elastic properties of nanomaterials and should be considered while designing materials for high-temperature applications. The variation of bulk modulus with temperature for nanomaterials such as Fullerene (C_{60}), Ni, Ag, TiO_2 , Al, and Cu are shown in Figure 7 to Figure 12. Among the examined nanomaterials, Fullerene (C_{60}) demonstrates the most severe fall in bulk modulus at higher temperatures, indicating a stronger temperature dependence. On the other hand, nanocrystalline Ag, TiO_2 , Al, and Cu exhibit a roughly linear decline, indicating relatively constant mechanical performance over the temperature range under investigation. The findings unequivocally show that temperature has a substantial impact on the elastic characteristics of nanomaterials, however the degree of this impact varies depending on the type of material. Overall, the patterns reported are physically consistent with the expected behavior of solids and verify that nanoparticles soften with increasing temperature. These results are helpful in choosing appropriate nanomaterials for high-temperature engineering and nano-device applications, where mechanical stability is crucial.

Figure 13 to Figure 18 demonstrates the fluctuation of pressure with volume expansion ratio $\left(\frac{V}{V_0} \right)$ for Fullerene (C_{60}), Ni, Ag, TiO_2 , Al, and nanocrystalline Cu computed using the Murnaghan Equation of State (MEOS) and Tait Equation of State (TEOS). For all examined nanomaterials, pressure reduces constantly with increasing volume expansion, showing the creation of tensile (negative) pressure during thermal expansion. Although numeric variations are noted, both equations of state predict the same qualitative behavior. For the same volume expansion ratio, the Tait EOS consistently forecasts larger negative pressure values than the Murnaghan EOS, indicating a comparatively higher sensitivity of TEOS to volume changes. The authors report the relative deviation between TEOS and MEOS in Table 3. The discrepancy arises from the different mathematical formulations of the pressure-volume relationship in TEOS and MEOS. The pressure-volume curves were used to analyze the relative deviation between TEOS and MEOS. Because of their differing pressure-volume formulations and the ensuing nonlinear response in the enlarged state, TEOS forecasts slightly higher negative (tensile) pressures than MEOS, especially at larger volume expansions. When thermal expansion raises the volume above the reference volume, MEOS and TEOS directly provide the

negative pressure. Instead of an externally supplied tensile load, it represents a tensile hydrostatic pressure obtained from EOS. The pressure-volume formulas of TEOS and MEOS differ from one another. At higher volume expansion ratios, the difference between the two models becomes more noticeable. Aluminum (Al) shows the biggest pressure fluctuation with volume expansion among the nanomaterials under study, while nanocrystalline Cu and Ag show relatively smaller pressure variations because of their lower thermal expansion. Because of its unique molecular structure and great compressibility, fullerene (C_{60}) exhibits a nonlinear reduction in pressure. Over the studied range, Ni and TiO_2 show intermediate behavior with almost linear pressure-volume correlations. Overall, the results reveal that both MEOS and TEOS successfully explain the pressure-volume expansion behavior of nanomaterials. However, the Tait EOS is more sensitive for simulating thermal expansion effects in nanomaterials since it predicts somewhat higher tensile stresses than the Murnaghan EOS, particularly at higher volume expansion. The model treats $\alpha(T)$ as temperature-dependent while using room-temperature B_0 and B'_0 as reference parameters. Accuracy may be limited at higher temperatures because B_0 and other thermoelastic parameters are not explicitly temperature dependent. The manuscript makes this restriction clear.

4. Conclusions

The thermal expansion behavior of Fullerene (C_{60}), 20 nm Ni, nanocrystalline Ag, TiO_2 , Al, and Cu nanoparticles was effectively examined using the Murnaghan equation of state (MEOS) and the Tait equation of state (TEOS). The computed normalized volume expansion $\left(\frac{V}{V_0} \right)$ increases monotonically with temperature for all examined nanomaterials, corresponding with the expected physical behavior. The outstanding match between the present results and the theoretical predictions shows the validity and trustworthiness of the suggested model. Additionally, the results' agreement with Fang et al.'s theoretical model shows that the current method correctly forecasts the thermal expansion behavior with a small number of input factors. Owing to its simplicity, computational efficiency, and high predictive accuracy, the proposed formulation can serve as a reliable tool for evaluating the thermal expansion properties of a wide range of nanomaterials.

The computed results by using equation -13 demonstrate that thermal expansion and weakening of interatomic forces cause the bulk modulus of all examined nanomaterials to decrease with increasing temperature. while Ag, TiO_2 , Al, and Cu show almost linear and progressive bulk modulus declines, fullerene (C_{60}) shows the highest temperature sensitivity. The work demonstrates that temperature significantly affects nanoparticles' elastic characteristics and should be taken into account when creating materials for high-temperature applications.

The pressure reduces monotonically with increasing volume expansion for all nanomaterials. The Tait EOS regularly forecasts higher negative pressures than the Murnaghan EOS, despite the fact that both equations show comparable trends. This demonstrates that both EOS models are suitable for explaining thermoelastic behavior, whereas TEOS provides a stronger prediction of tensile pressure during thermal expansion. Instead of utilizing a particle-size-dependent model, the current work concentrates on temperature-dependent thermal expansion using Murnaghan and Tait EOS. Size-dependent elastic characteristics, surface and grain-boundary effects, and size-dependent thermal expansion have been recognized as limits and are recommended to be taken into account in subsequent research.

Abbreviations

EOS	Equation of State
TEOS	Tait Equation of State
MEOS	Murnaghan Equation of State
AgNPs	Silver Nanoparticles

Author Contributions

Rajendra Kumar Mishra: Conceptualization, Formal Analysis, Investigation, Methodology, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing

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Conflicts of Interest

The authors declares no conflicts of interest.

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