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Enhancing the Order of Compression Significantly Improves the Accuracy of the Equation of State, Leading to More Reliable Predictions and Insights

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Abstract: This study presents a new, innovative exponential equation of state (EOS) that can be applied in different orders, from first through fourth, aiming to improve prediction accuracy across various levels of material compression. The significance of this new exponential EOS lies in its ability to accurately predict material behaviour under high compression, a crucial aspect in high-pressure physics. A thorough and detailed analysis compares this new exponential EOS to the well-known fourth-order Birch-Murnaghan EOS. The comparison shows that the exponential EOS matches and often outperforms the Birch-Murnaghan EOS, especially at higher compression levels. This is particularly important because the fourth-order exponential EOS proves highly accurate for materials like hexagonal close-packed (HCP) iron and sodium halides under high compression. In contrast, while the Birch-Murnaghan EOS performs adequately at lower compressions, it tends to deviate from experimental data as compression increases.Additionally, the study reviews the Shanker EOS. It acknowledges the work of M. Kumar and colleagues, who noted its limitations at high compression levels and proposed necessary parameter adjustments for different materials. These issues have been addressed by the new fourth-order exponential EOS, which is more adaptable and provides consistent and reliable results across both low and high-compression ranges, making it a valuable tool in high-pressure physics.

Keywords: Equation of State, Carbon nanotubes, Compression, Thermal pressure, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS.

Introduction:

The equation of state (EOS) is an essential tool in physics and engineering, defining the mathematical relationships between key state variables like pressure, volume, and temperature [1-3]. These relationships are critical for understanding how different substances and systems behave, from simple gases to complex fluids. With advancing technology and the growing need for precise predictions, improving the accuracy of EOS models for solids has become more critical than ever. Our research shows that increasing compression improves EOS accuracy, and we aim to explore how higher compression levels affect EOS precision. Specifically, we want to see how adding higher-order corrections, which are additional terms in the EOS that account for more complex interactions between particles, influences the predictive accuracy of the EOS and identifies the level of compression beyond which further refinement offers limited benefit [4-8].

This study responds to the demand for more accurate EOS models in fields like materials science, astrophysics, and industrial processes, offering a valuable tool to practitioners in these areas. In the following sections, we review current EOS and compression techniques, lay out the theoretical basis for higher-order compression, and describe our approach to assessing EOS accuracy. We will examine the benefits and limitations of raising the compression order using analytical and computational methods. Finally, we discuss our findings and their implications for future research and practical applications. Our research not only enhances our theoretical understanding of high-pressure physics but also has practical implications for industries and fields that rely on accurate EOS models for their operations.

Our research analyses the effects of higher-order compression on EOS accuracy and reliability, aiming to improve model precision and support better decision-making in scientific and engineering fields. This study covers various levels of EOS compression, including third-order compression in the Srivastava-Pandey EOS, first-order compression in the Murnaghan EOS, second-order compression in the Kholiya EOS, and unspecified higher-degree compression in the Usual-Tait EOS.

Method of Analysis:

To analyse the compression-dependent properties of carbon nanotubes, we have considered equations of state such as:

The Srivastava-Pandey EOS is a valuable framework for improving predictions of material properties beyond standard models, especially when considering the influence of nanoscale effects and high-strain conditions. The Srivastava-Pandey EOS[18] is expressed as:

$$P=\left[\frac{B_0}{\alpha^4}\left(\frac{V}{V_0}\right)^{-4/3}\right]\times\left[\left\{\alpha^3(1+z+z^2+z^3)+\alpha^2(-3z^2-2z-1)+\alpha(6z+2)-6\right\}e^{\alpha z}-(\alpha^3-\alpha^2+2\alpha-6)\right] \quad (1)$$

Where, $z = 1 - \frac{V}{V_0}$ and $\alpha = \frac{3K_0^{'} - 8}{3}$.

The Murnaghan Equation of State (EOS) describes the relationship between pressure, volume, and compressibility in solids under high pressure. It assumes a linear dependence of bulk modulus on pressure and is widely used to model materials' behaviour in geophysics and condensed matter physics due to its simplicity and accuracy. The Murnaghan EOS [19] can be expressed as:

$$P = \frac{B_0}{B_{0'}^{'}}\left[\left(\frac{V}{V_0}\right)^{-B_0^{'}} - 1\right] \quad (2)$$

The Kholiya Equation of State (EOS) is a thermodynamic model used to predict the behaviour of nanomaterials under high pressure, focusing on their compression properties. This EOS is mainly applied to describe the volume changes in materials at nanoscale dimensions, using input parameters like the bulk modulus and its pressure derivative. It is a variant of the more common Tait EOS and, in some cases, is considered a limiting form of Tait's equation. While it offers decent accuracy, it may deviate slightly from other models, such as Murnaghan and Vinet, at high pressures. The Khoya EOS [20] can be expressed as:

$$P = \frac{K_0}{2}\left[\left(K_0^{'} - 3\right) - 2\left(K_0^{'} - 2\right)\left(\frac{V}{V_0}\right)^{-1} + \left(K_0^{'} - 1\right)\left(\frac{V}{V_0}\right)^{-2}\right] (3)$$

The Usual Tait EOS models the relationship between pressure and compression, assuming that the product of thermal expansion and bulk modulus remains constant under pressure. It's widely applied to liquids and solids. The Usual-Tait EOS [21] can be expressed as:

$$P = \frac{K_0}{\left(K_0^{'} + 1\right)}\left[\exp\left\{\left(K_0^{'} + 1\right)\left(1 - \frac{V}{V_0}\right)\right\} - 1\right] \quad (4)$$

Bulk Modulus:

The first volume derivative of isothermal EOS gives Isothermal Bulk modulus (K_T) gives as

$$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T \quad (5)$$

Also, the expression for the first pressure derivative of isothermal bulk modulus can be obtained by the following expression;

$$K_T^{'} = \left(\frac{\partial K_T}{\partial P}\right)_T = \left(\frac{\partial K_T}{\partial V}\right)_T \cdot \left(\frac{\partial V}{\partial P}\right)_T$$

(6)

The expression for the bulk modulus can be obtained by using equation (5) with different equations of state, such as the Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS.

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-1/3}\left(1+z+z^2+z^3\right)\exp\left(\alpha z\right)+\frac{4}{3}P \quad (7)$$

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-K_0'}$$

(8)

$$K_T = K_0\left(K_0'-2\right)\left(\frac{V}{V_0}\right)^{-1}\left[\left(\frac{K_0'-1}{K_0'-2}\right)\left(\frac{V}{V_0}\right)^{-1}-1\right]$$

(9)

$$K_T = K_0\left(\frac{V}{V_0}\right)\exp\left\{\left(K_0'+1\right)\left(1-\frac{V}{V_0}\right)\right\}$$

(10)

The first-order pressure derivatives of bulk modulus are expressed usingequation(6) across various equations of state, including the Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS.

$$K_T' = \left(1-\frac{4P}{3K_T}\right)\left(\frac{1}{3}+\frac{V}{V_0}\left\{\alpha+\frac{\left(1+2z+3z^2\right)}{\left(1+z+z^2+z^3\right)}\right\}\right)+\frac{4}{3}$$

(11)

$$K'_T = \frac{K_0K_0'}{K_T}\left(\frac{V}{V_0}\right)^{-K_0'}$$

(12)

$$K_T' = \frac{\left(K_0'-2\right)\left(\frac{V}{V_0}\right)-2\left(K_0'-1\right)}{\left(K_0'-2\right)\left(\frac{V}{V_0}\right)-\left(K_0'-1\right)} \quad (13)$$

$$K_T' = \left(K_0'+1\right)\left(\frac{V}{V_0}\right)-1$$

(14)

Volume Thermal Expansion Coefficient:

The product of the volumetric thermal expansion coefficient (α) and isothermal bulk modulus (K_T) is a proven and unchanging constant for all solids. This scientific principle has been extensively studied and verified by experts in the field. By knowing and confidently applying this principle, we can gain deeper insights into the behaviour of materials under varying temperature and pressure conditions and open new pathways to advances in material science.

$\alpha K_T = \text{Constant}$

Shanker and Kumar show that:

$$\alpha K_T = \alpha_0 K_0$$

$$\alpha = \alpha_0 \left(\frac{K_0}{K_T} \right)$$

$$\alpha_r = \frac{\alpha}{\alpha_0} = \frac{K_0}{K_T}$$

(15)**Table 1:**Input parameters K_0 (GPa) and K_0', For carbon nanotube bundles and individual.

Materials	Ko (GPa)	Ko'
Carbon nanotubes bundles	37 [22, 23]	11[22, 23]
Carbon nanotubes Individuals	230[22,23]	4.5 [22, 23]

Table 2: Calculated pressure values for bundles and individual carbon nanotubes concerning varying compression by Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS with experimental data.

V/V_0	P(S-P)	P (M)	P (K)	P (U-T)	P (Exp.) [22-23]	V/V_0	P(S-P)	P (M)	P (K)	P (U-T)	P (Exp.) [22-23]
1	0.0	0.0	0.0	0.0	0.0	1	0.0	0.0	0.0	0.0	0.0
0.9769	1.0	1.0	1.0	1.0	1.0	0.9944	1.3	1.3	1.3	1.3	1.0
0.9638	1.7	1.7	1.7	1.7	1.5	0.9925	1.8	1.8	1.8	1.8	1.5
0.9513	2.4	2.5	2.4	2.4	2.0	0.9900	2.4	2.4	2.4	2.4	2.0
0.9425	3.0	3.1	2.9	3.1	2.5	0.9888	2.7	2.7	2.6	2.7	2.5
0.9400	3.2	3.3	3.1	3.3	3.0	0.9863	3.3	3.3	3.3	3.3	3.0
0.935	3.6	3.7	3.5	3.6	3.5	0.9838	3.9	3.9	3.9	3.9	3.5
0.9238	4.6	4.7	4.3	4.6	4.0	0.9825	4.2	4.2	4.2	4.2	4.0
0.9213	4.8	4.9	4.5	4.8	4.5	0.9800	4.9	4.9	4.8	4.9	4.5
0.9188	5.0	5.2	4.7	5.1	5.0	0.9781	5.4	5.4	5.3	5.4	5.0
0.9088	6.1	6.3	5.6	6.1	5.5	0.9776	5.5	5.5	5.4	5.5	5.5
0.9063	6.3	6.6	5.8	6.4	6.0	0.9757	6.0	6.0	5.9	6.0	6.0
0.8981	7.3	7.6	6.6	7.4	6.5	0.9738	6.5	6.5	6.4	6.5	6.5
0.8963	7.5	7.9	6.8	7.6	7.0	0.972	7.0	7.0	6.9	7.0	7.0
0.8900	8.3	8.8	7.4	8.5	7.5	0.9702	7.4	7.5	7.4	7.4	7.5
0.8875	8.7	9.1	7.7	8.8	8.0	0.9683	8.0	8.0	7.9	8.0	8.0
RMSD	46.2	14.1	7.8	11.8		RMSD	11.4	11.6	74.2	11.6	

Table 3. Calculated bulk modulus values for bundles and individual carbon nanotubes concerning varying compression by Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS.

V/V_o	K_T (S-P)	K_T (M)	K_T (K)	K_T (U-T)	V/V_o	K_T (S-P)	K_T (M)	K_T (K)	K_T (U-T)
1.0000	37.0	37.0	37.0	37.0	1.0000	230.0	230.0	230.0	230.0
0.9769	47.6	47.8	46.8	47.7	0.9944	235.9	235.9	235.9	235.9
0.9638	54.8	55.5	52.8	55.1	0.9925	237.9	237.9	237.9	237.9
0.9513	62.5	64.1	58.8	63.1	0.9900	240.6	240.6	240.5	240.6
0.9425	68.7	71.0	63.2	69.5	0.9888	241.9	242.0	241.8	241.9
0.9400	70.5	73.1	64.5	71.5	0.9863	244.6	244.7	244.5	244.6
0.9350	74.4	77.5	67.1	75.5	0.9838	247.3	247.5	247.3	247.4
0.9238	83.7	88.5	73.1	85.3	0.9825	248.8	249.0	248.7	248.8
0.9213	85.9	91.2	74.5	87.6	0.9800	251.6	251.9	251.5	251.6
0.9188	88.2	93.9	75.9	90.1	0.9781	253.8	254.1	253.6	253.8
0.9088	98.0	105.9	81.6	100.5	0.9776	254.3	254.7	254.1	254.3
0.9063	100.5	109.2	83.0	103.2	0.9757	256.5	256.9	256.3	256.5
0.8981	109.5	120.7	87.9	112.9	0.9738	258.7	259.2	258.4	258.7
0.8963	111.6	123.4	89.0	115.1	0.9720	260.8	261.4	260.5	260.8
0.8900	119.1	133.3	93.0	123.3	0.9702	262.8	263.5	262.5	262.9
0.8875	122.4	137.5	94.5	126.7	0.9683	265.1	265.9	264.7	265.1

Table 4. Calculated values of first pressure derivative of bulk modulus for bundles and individual carbon nanotubes concerning varying compression by Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS.

V/V_o	K'_T(S-P)	K'_T(M)	K'_T(K)	K'_T(U-T)	V/V_o	K'_T(S-P)	K'_T(M)	K'_T(K)	K'_T(U-T)
1.0000	1.000	11.000	11.000	11.000	1.0000	4.500	4.500	4.500	4.500
0.9769	0.977	10.542	11.000	9.279	0.9944	4.467	4.500	4.452	4.469
0.9638	0.964	10.311	11.000	8.543	0.9925	4.454	4.500	4.436	4.459
0.9513	0.951	10.120	11.000	7.953	0.9900	4.440	4.500	4.415	4.445
0.9425	0.943	9.985	11.000	7.590	0.9888	4.433	4.500	4.405	4.438
0.9400	0.940	9.945	11.000	7.494	0.9863	4.418	4.500	4.384	4.425
0.9350	0.935	9.868	11.000	7.309	0.9838	4.404	4.500	4.364	4.411
0.9238	0.924	9.702	11.000	6.932	0.9825	4.397	4.500	4.353	4.404
0.9213	0.921	9.671	11.000	6.854	0.9800	4.382	4.500	4.333	4.390
0.9188	0.919	9.642	11.000	6.778	0.9781	4.371	4.500	4.318	4.380
0.9088	0.909	9.498	11.000	6.492	0.9776	4.369	4.500	4.314	4.377
0.9063	0.906	9.474	11.000	6.425	0.9757	4.358	4.500	4.300	4.366
0.8981	0.898	9.364	11.000	6.216	0.9738	4.347	4.500	4.285	4.356
0.8963	0.896	9.343	11.000	6.173	0.9720	4.337	4.500	4.271	4.346
0.8900	0.890	9.266	11.000	6.025	0.9702	4.328	4.500	4.257	4.336
0.8875	0.888	9.230	11.000	5.969	0.9683	4.317	4.500	4.243	4.326

Table 4. Calculated values of the relative isothermal expansion coefficients for bundles and individual carbon nanotubes under varying compression using the Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS.

V/V_o	α_r(S-P)	α_r(M)	α_r(K)	α_r(U-T)	V/V_o	α_r(S-P)	α_r(M)	α_r(K)	α_r(U-T)
1.0000	1.000	1.000	1.000	1.000	1.0000	1.000	1.000	1.000	1.000
0.9769	0.777	0.773	0.790	0.776	0.9944	0.975	0.975	0.975	0.975
0.9638	0.675	0.667	0.701	0.672	0.9925	0.967	0.967	0.967	0.967
0.9513	0.592	0.577	0.629	0.586	0.9900	0.956	0.956	0.956	0.956
0.9425	0.539	0.521	0.585	0.532	0.9888	0.951	0.951	0.951	0.951
0.9400	0.525	0.506	0.574	0.518	0.9863	0.940	0.940	0.941	0.940
0.9350	0.498	0.477	0.552	0.490	0.9838	0.930	0.929	0.930	0.930
0.9238	0.442	0.418	0.506	0.434	0.9825	0.925	0.924	0.925	0.924
0.9213	0.431	0.406	0.497	0.422	0.9800	0.914	0.913	0.915	0.914
0.9188	0.420	0.394	0.488	0.411	0.9781	0.906	0.905	0.907	0.906
0.9088	0.378	0.349	0.454	0.368	0.9776	0.904	0.903	0.905	0.904
0.9063	0.368	0.339	0.446	0.358	0.9757	0.897	0.895	0.897	0.897
0.8981	0.338	0.307	0.421	0.328	0.9738	0.889	0.887	0.890	0.889
0.8963	0.332	0.300	0.416	0.321	0.9720	0.882	0.880	0.883	0.882
0.8900	0.311	0.278	0.398	0.300	0.9702	0.875	0.873	0.876	0.875
0.8875	0.302	0.269	0.391	0.292	0.9683	0.868	0.865	0.869	0.868

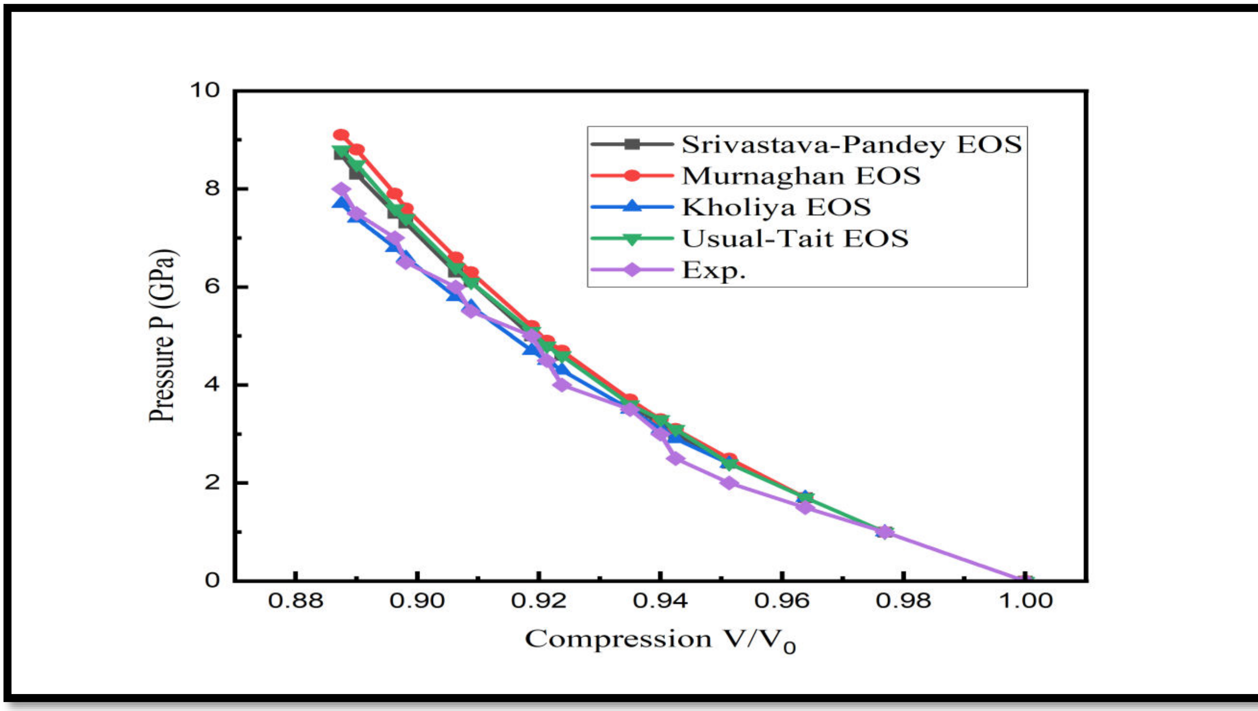

Fig. 1: Pressure versus Compression for Carbon nanotube bundle

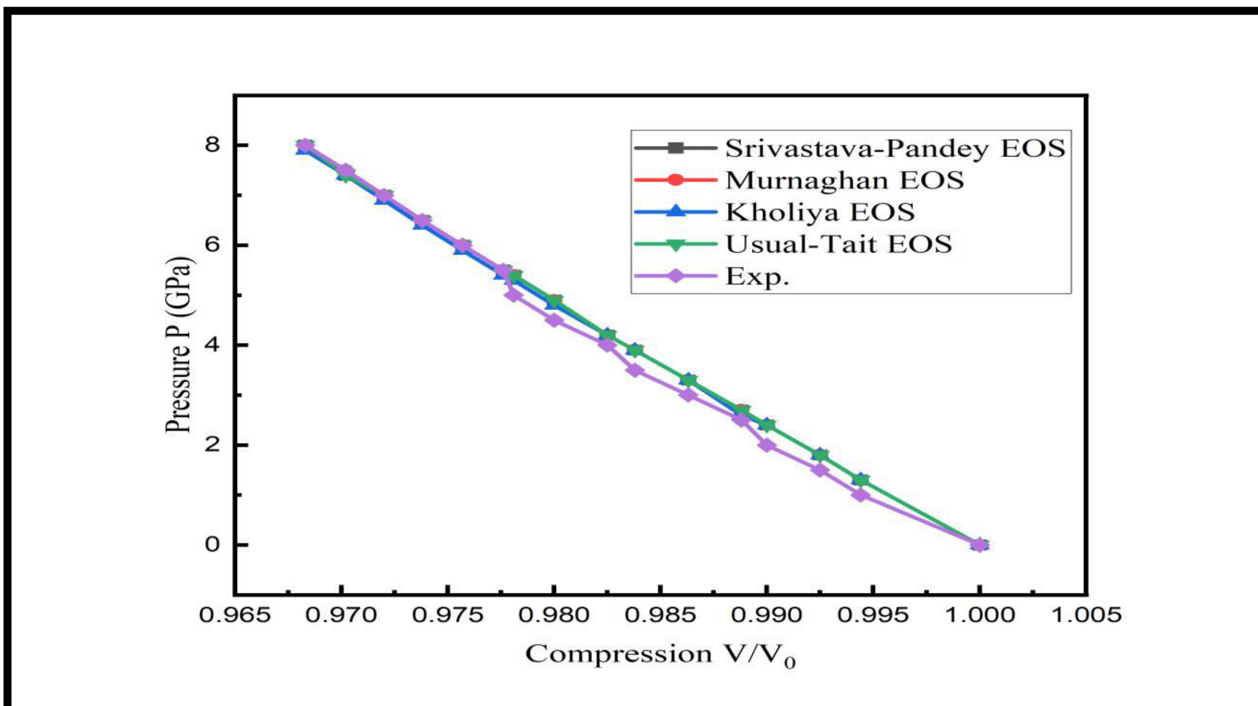

Fig. 2: Pressure versus Compression for Carbon nanotube individual

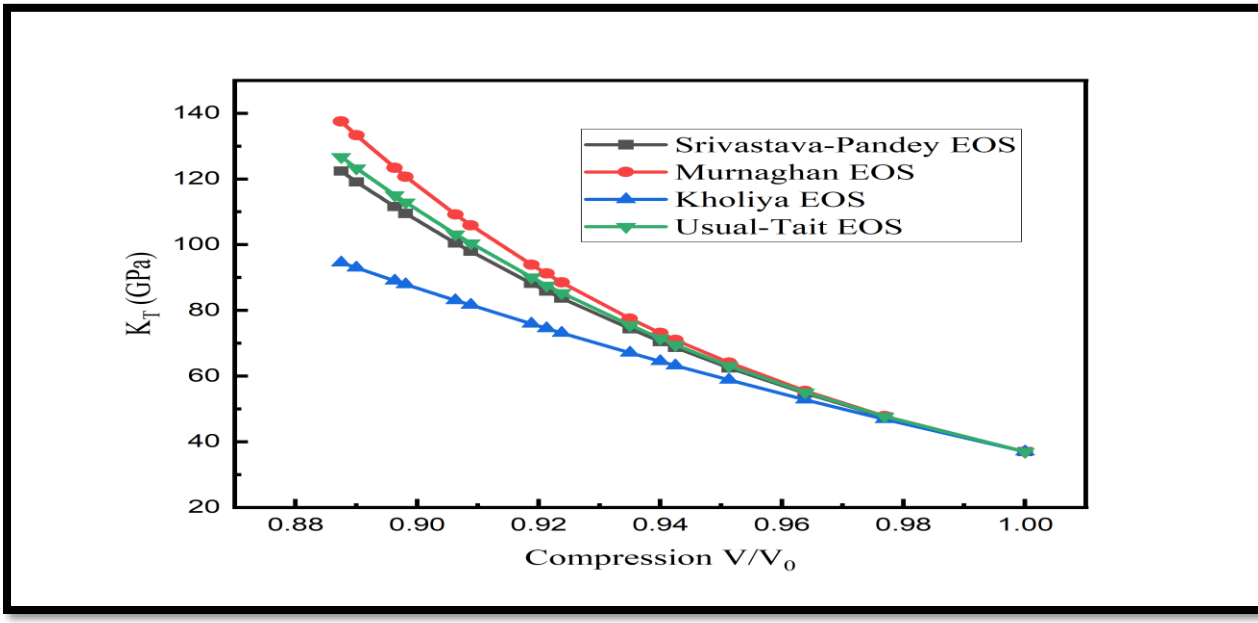

Fig. 3: Compression-dependent bulk modulus of Carbon nanotube bundle

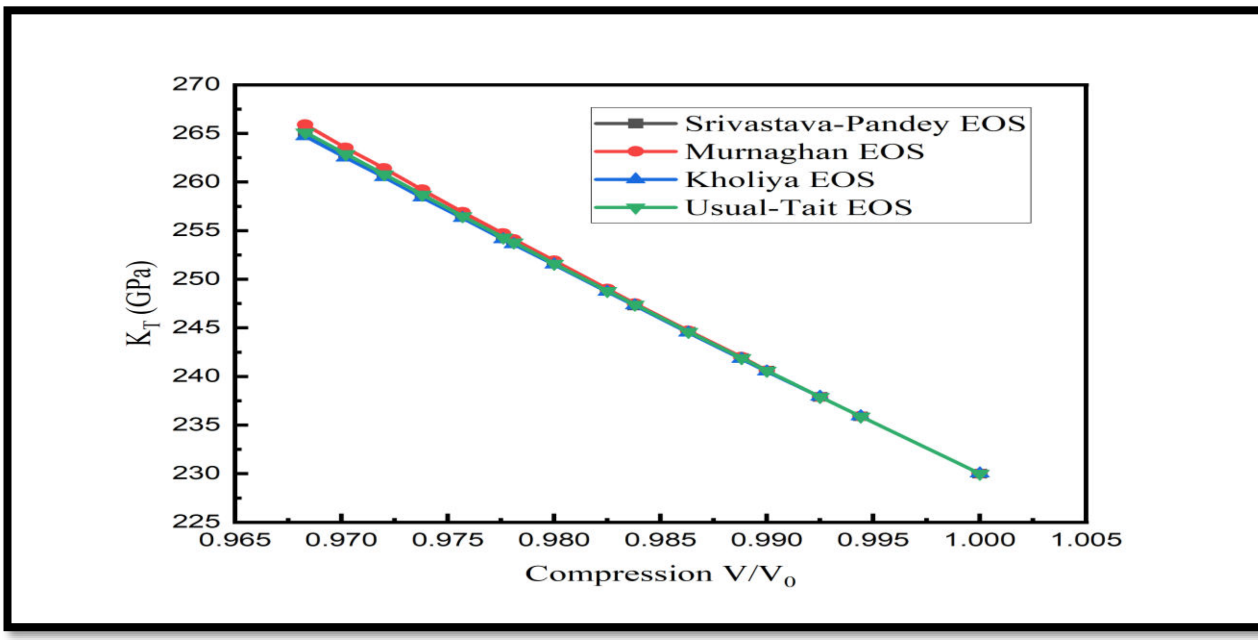

Fig. 4: Compression-dependent bulk modulus of Carbon nanotube individual.

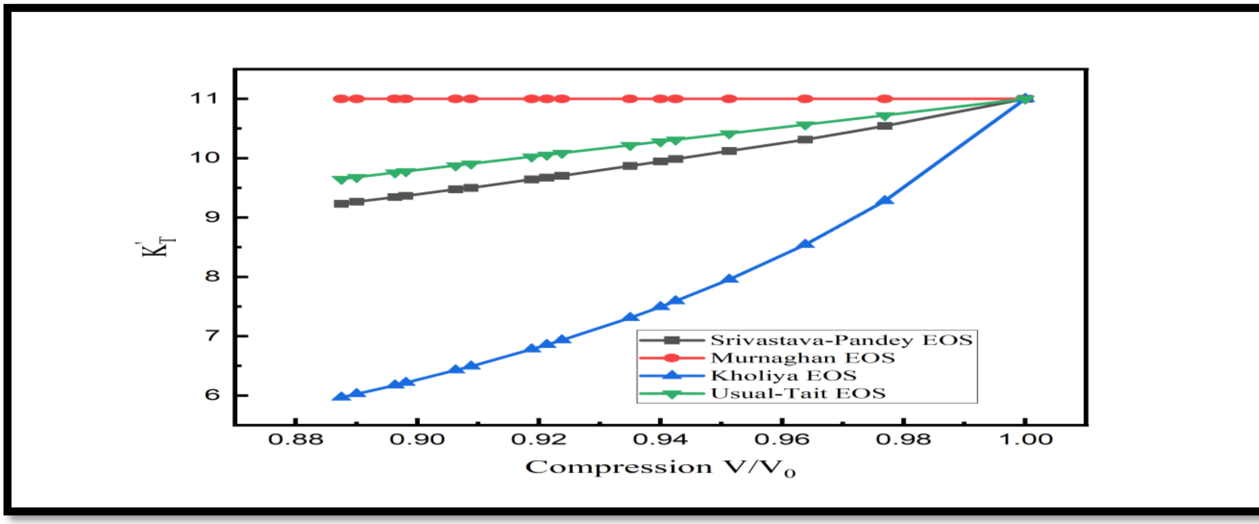

Fig. 5: Compression dependent first order pressure derivative of bulk modulus of Carbon nanotube bundle.

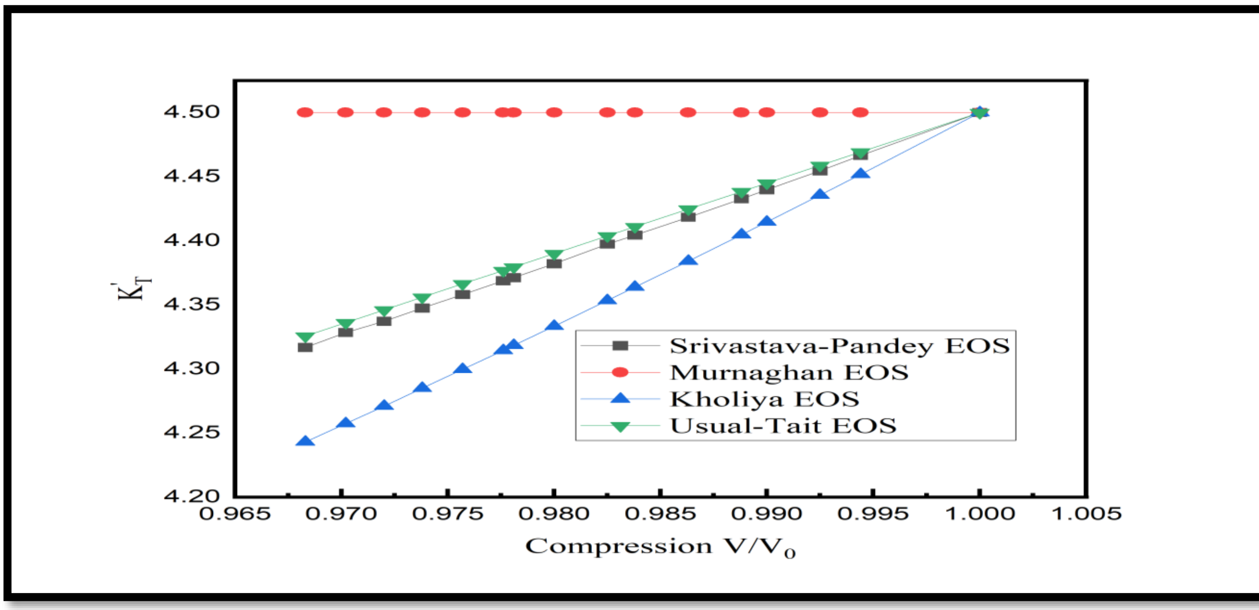

Fig. 6: Compression dependent first order pressure derivative of bulk modulus of Carbon nanotube individual

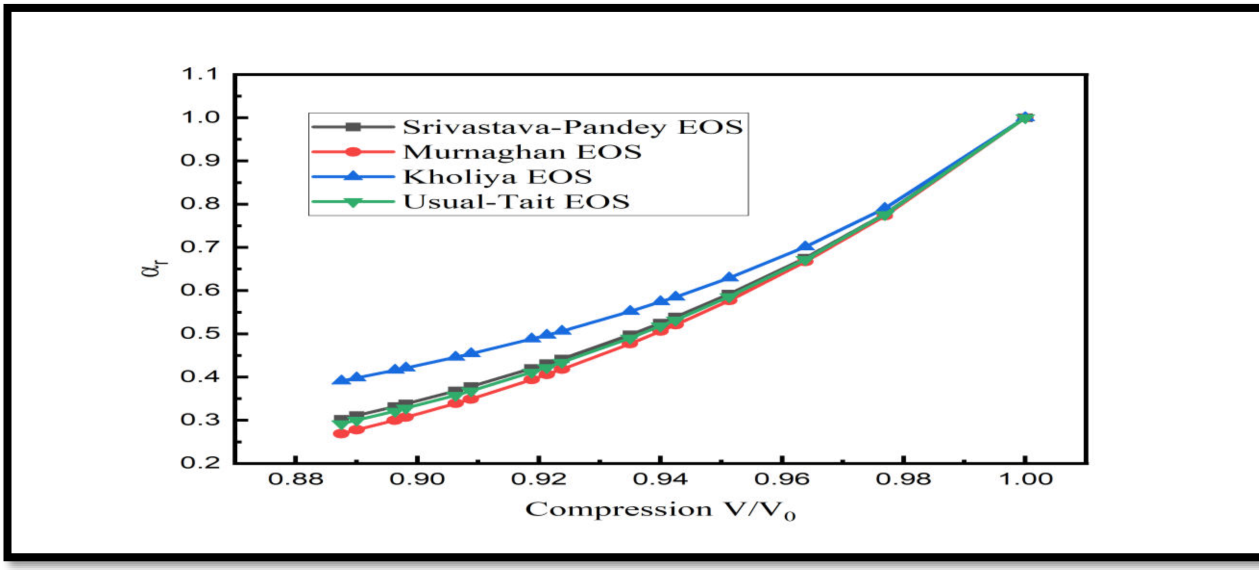

Fig. 7: Compression-dependentrelative volume thermal expansion coefficient of Carbon nanotube bundle

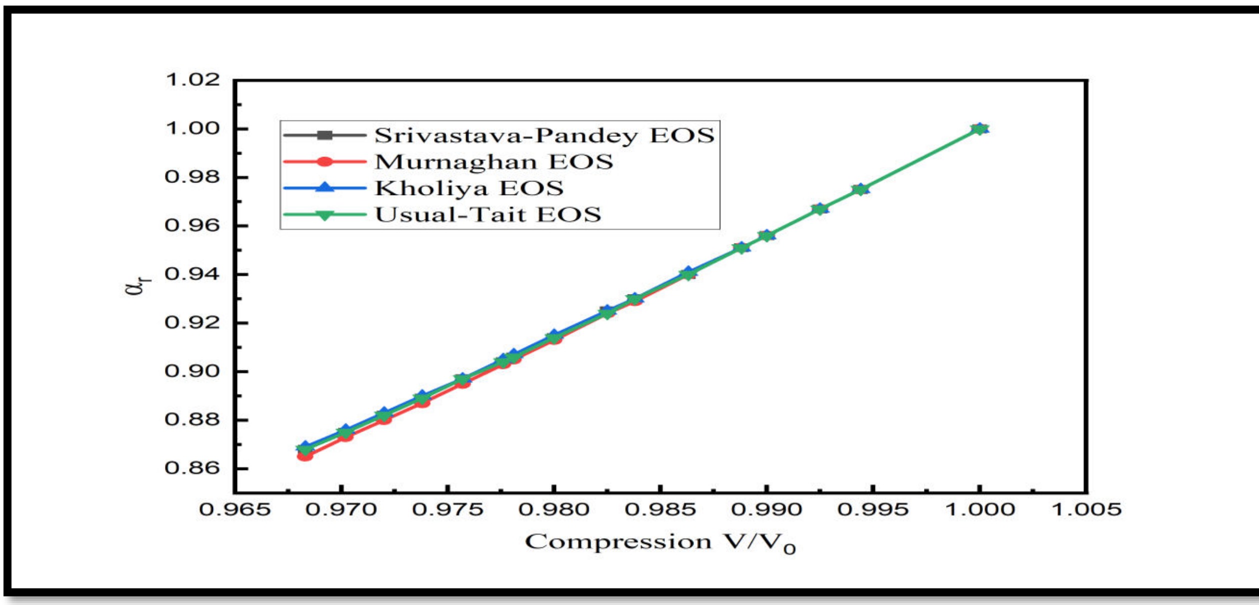

Fig. 8: Compression-dependentrelative volume thermal expansion coefficient of carbon nanotube individual.

Result and Discussion:

The analysis is based on four widely used equations of state: Srivastava-Pandey EOS, Murnaghan EOS, Kholiya EOS, and Usual-Tait EOS, each representing different orders of compressions. The Srivastava-Pandey EOS is well-suited for complex materials under extreme conditions, while the Usual-Tait EOS effectively handles liquids and solids based on superficial pressure-compression relationships. The Murnaghan EOS is optimal for solids under moderate pressure, and the Kholiya EOS specialises inmodelling nanomaterials under high-pressure conditions. We calculated values for pressure (P), bulk modulus, the first-order pressure derivative of bulk modulus, and the relative isothermal volume thermal expansion coefficient at different compression levels for both bundled and individual nanotubes.

Table 1 presents the input parameters for bundles and individual carbon nanotubes. The calculated values using the Srivastava-Pandey, Murnaghan, Kholiya, and Usual-Tait equations of state are shown in Tables 2-4.

The curves illustrate the relationships between compression and pressure, compression and bulk modulus, compression and the first-order derivative of bulk modulus, and compression and the relative volume thermal expansion coefficient, as depicted in Figures 1-8.

Data from Table 1 and Figures 1-2 indicate that the results from the Kholiya formulation do not align with the experimental data. Conversely, the results from the Murnaghan, Usual-Tait, and Srivastava-Pandey equations of state closely match the experimental data. However, all equations yield similar outcomes at low compression. The Kholiya equation provides lower results than the experimental curve at high compression. In contrast, the Srivastava-Pandey and Usual-Tait equations produce results slightly above the experimental curve, exhibiting minor deviations. The Murnaghan equation shows the most significant deviation for bundled carbon nanotubes, while the results for individual nanotubes remain roughly similar, except for slight deviations noted in the Kholiya equation.

Analysing the data from Tables 2 and 3 and Figures 3-6 reveals that the bulk modulus increases with the rising compression. In contrast, the first-pressure derivative of the bulk modulus decreases with increased compression. For bundled carbon nanotubes, the Usual-Tait and Srivastava-Pandey equations yield similar results but show higher degrees of compression. The Kholiya equation deviates in the lower region of the curve, while the Murnaghan equation deviates in the upper area. All equations exhibit comparable results for individual nanotubes, although the Kholiya and Murnaghan equations show slight deviations from the Usual-Tait and Srivastava-Pandey equations.

In the case of bundled nanotubes, the first-order pressure derivative of the bulk modulus calculated using the Kholiya equation shows maximum deviation due to its basis on the virial equation while considering only the second-order term. Although the results deviate from other equations, those obtained from the Murnaghan equation remain consistent regardless of compression.

The graphs in Figures 7-8 indicate that the relative volume thermal expansion coefficient decreases as compression increases. This trend holds for individual nanotubes, but a deviation occurs for bundled nanotubes when using the Kholiya EOS. After analysing the data, we conclude that equations derived with a higher degree of compression are better suited for predicting the thermoelastic properties of nano-objects compared to those derived with a lower degree of compression. The essential result of this analysis is that the" higher order equation of state is more effective for that element having high value of bulk modulus, but for low values of bulk modulus, lower order is better than higher orders.

Conclusion:

After carefully analysing the available descriptions, we found that the equation of state, which accounts for higher degrees of compression, is more effective in predicting the thermoelastic properties of nanomaterials and nanoobjects under conditions of high compression. In contrast, alternative equations of state are only suitable for low compression scenarios since they only consider lower degrees of compression.By enhancing the order of compression, we can significantly improve the accuracy of the equation of state, which will provide us with more reliable predictions and insights.

Ethical Approval:

The authors confirm that the manuscript is original and unpublished.

Competing interests:

The authors of this paper declare no known financial interests or personal relationships that could have affected the presented work.

Author's Contribution:

All the authors collaborated to create the research outline. Abhay P Srivastava performed all the necessary calculations and drafted the initial manuscript. Professor B. K. Pandey provided resources and guidance throughout the project. Finally, Dr. Anjani K Pandey reviewed and edited the final draft.

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References:

1. M. Abbaspour, H. Akbarzadeh, S. Salemi, and M. Abroodi, "Equation of state and some structural and dynamical properties of the confined Lennard-Jones fluid into carbon nanotube: A molecular dynamics study," Physica A: Statistical Mechanics and its Applications, vol. 462, pp. 1075–1090, Nov. 2016.
2. J. Shanker and B. P. Singh, "A comparative study of Keane's and Stacey's equations of state," Physica B: Condensed Matter, vol. 370, no. 1–4, pp. 78–83, Dec. 2005.
3. A. P. Srivastava, B. K. Pandey, A. K. Gupta, and A. K. Pandey, "A New Approach to Evaluate Pressure of Solids at High Compression," National Academy Science Letters, Jun. 2024.
4. R. Kishore, "Generalized equations for the steady-state analysis of inhomogeneous semiconductor devices," Solid-State Electronics, vol. 33, no. 8, pp. 1049–1054, Aug. 1990.
5. J. Patel, J. Gupta, A. P. Srivastava, M. Upadhyaya, and B. K. Pandey, "A theoretical equation of state to formulate the melting curve of metals with varying pressure," Computational Condensed Matter, vol. 40, p. e00921, Sep. 2024.
6. R. S. Chauhan and C. P. Singh, "Analysis of melting for alkali halides based on the potential energy curve," Physica B: Condensed Matter, vol. 324, no. 1–4, pp. 151–156, Nov. 2002.
7. K. Sunil, M. P. Singh, and B. S. Sharma, "Analysis of melting behaviour of some transition metals at high pressures," Computational Condensed Matter, vol. 35, p. e00813, Jun. 2023.
8. S. Kumar, R. Kumar, R. P. Agarwal, and B. Samet, "A study of fractional Lotka-Volterra population model using Haar wavelet and Adams-Bashforth-Moulton methods," Mathematical Methods in the Applied Sciences, vol. 43, no. 8, pp. 5564–5578, May 2020.
9. S. Cho et al., "Interfacial analysis of TiO 2 coated carbon nanofibers and Mg-Al alloy matrix fabricated using a liquid pressing process," Scripta Materialia, vol. 136, pp. 50–54, Jul. 2017.
10. C. M. Nandanwar, N. S. Kokode, R. M. Yerojwar, and A. N. Yerpude, "Combustion synthesis and photoluminescence study of novel Sm3+ activated K3La(PO4)2 phosphor for n-UV solid-state lighting," Nano-Structures & Nano-Objects, vol. 36, p. 101068, Oct. 2023.
11. E. V. Kumaret al., "Facile green synthesis of Cu-doped MoO3 nanoparticles and its application for the photocatalytic degradation of hazardous organic pollutants," Nano-Structures & Nano-Objects, vol. 36, p. 101066, Oct. 2023.

12. M. Zhou, W. Zhu, S. Yu, Y. Tian, and K. Zhou, "Selective laser sintering of carbon nanotube–coated thermoplastic polyurethane: Mechanical, electrical, and piezoresistive properties," Composites Part C: Open Access, vol. 7, p. 100212, Mar. 2022.
13. M. Zhong, M. Zhang, and X. Li, "Carbon nanomaterials and their composites for supercapacitors," Carbon Energy, vol. 4, no. 5, pp. 950–985.
14. I. Khan, K. Saeed, and I. Khan, "Nanoparticles: Properties, applications and toxicities," Arabian Journal of Chemistry, vol. 12, no. 7, pp. 908–931, Nov. 2019.
15. M. Goyal, "Melting temperature of metals under pressure," Chinese Journal of Physics, vol. 66, pp. 453–460, Aug. 2020.
16. N. B. Duc, H. K. Hieu, P. T. M. Hanh, T. T. Hai, N. V. Tuyen, and T. T. Ha, "Investigation of melting point, Debye frequency, and temperature of iron at high pressure," The European Physical Journal B, vol. 93, no. 6, p. 115, Jun. 2020.
17. S. Srivastava, P. Singh, A. K. Pandey, and C. K. Dixit, "Melting Temperature of Semiconducting Nanomaterials at different Shape and Size," Nano-Structures & Nano-Objects, vol. 36, p. 101067, Oct. 2023.
18. A. P. Srivastava, B. K. Pandey, A. K. Gupta, and M. Upadhyay, "The Relevance of the New Exponential Equation of State for Semiconductors," Iranian Journal of Science, Jun. 2024.
19. V. G. Tyuterev and N. Vast, "Murnaghan's equation of state for the electronic ground state energy," Computational Materials Science, vol. 38, no. 2, pp. 350–353, Dec. 2006.
20. P. Singh, B. K. Pandey, S. Mishra, and A. P. Srivastava, "Formulation for the prediction of melting temperature of metallic solids using suitable equation of states," Computational Condensed Matter, vol. 35, p. e00807, Jun. 2023.
21. K. Sunil, S. Rekha, S. Pushpendra, B.S. Sharma, A reinterpretation of the results for melting curves of metals based on the force – Heat equivalence energy density principle, Computational Condensed Matter, 38 (2024), e00862.
22. J. Chandra, P. K. Bhatt, and K. Kholiya, "Analysis of Equation of State for Carbon Nanotubes," Journal of Nanotechnology, vol. 2013, pp. 1–5, 2013.
23. S. Reich, J. Maultsch, C. Thomson and P. Ordejon, Raman Scattering in Carbon nanotubes revisited, Phys. Rev. B,**65(15),** 035412 (2002).