Investigation of Compression Behaviour of Bulk Inorganic Materials (Al, Cu, Pb, Ni, and Zn) Under High Pressure

Tajamul Islam[1*] A.K. Srivastava

[1]*Department of Chemical Engineering and Physical science, Lovely Professional University, Phagwara, Punjab, India-144411.*
**Corresponding Author: islam786physics@gmail.com*

KEYWORDS

Equation of State; Bulk Modulus; Compression; Volume.

ABSTRACT

This study investigates the compression behavior of aluminum (Al), copper (Cu), lead (Pb), nickel (Ni), and zinc (Zn) under varying pressure conditions, as predicted by several equations of state (EOS), including the Tait, Murnaghan, Kholiya and Chandra, and Shanker's equations. Each metal exhibits a consistent trend in volumetric compression (V/V_0) as pressure increases from 0 to 16 GPa, indicating a decrease in volume relative to the original volume (V/V_0). The Tait equation generally shows higher volumetric values at corresponding pressures compared to the other EOS models for all metals. In contrast, the Murnaghan equation provides values closely aligned with those from Kholiya and Chandra's equation, with minor deviations observed, particularly in nickel and zinc at higher pressures. Shanker's equation consistently predicts the lowest (V/V_0) values across all pressures for most metals, suggesting a more conservative estimate of volume reduction under compression. The data reveals the unique response of each metal to applied pressure, which is critical for applications in material science and engineering, providing insights into their mechanical properties and stability under extreme conditions. This comparative analysis enhances our understanding of the mechanical behavior of these metals, facilitating better material selection for high-pressure applications.

1. Introduction

High-pressure studies of bulk materials are always necessary because they shed light on the behavior of these materials under harsh circumstances, exposing phase transitions, structural deformations, and other crucial phenomena [1-5]. Mechanical features including volume compression and heat expansion are described by a variety of equations of state (EOS), including Tait's equation, Murnaghan's equation, Kholiya and Chandra Equation, and Shanker's equation of state [6-11]. The theoretical research of EOS at high pressure and high temperature are essentially significant enabling the extrapolation and interpolation into zones where experimental data is insufficient [12-13]. The equations of state (EOS) provide researchers with valuable perceptions into the properties of gases, liquids, and solids, enabling them to predict and analyze phase transitions, critical points, and other thermodynamic processes [14-15]. These equations serve as essential tools for understanding the behavior of matter under varying conditions, facilitating advancements in fields such as condensed matter physics and materials science [14-17]. Furthermore, the use of these EOS is essential for explaining how matter behaves in a variety of pressure, temperature, and volume situations [18-20]. Owing to their special qualities, inorganic metallic materials in bulk form play important roles in a variety of industries and technology [21–22]. These applications range from electrical components to structural materials [23-25]. It's crucial to remember that changes in economic conditions, environmental concerns, and technological improvements can all affect how useful these metals become over time [26-27].

As a result of changes in atomic and molecular organization, bulk materials studied under high pressure show a variety of alterations in their physical and chemical properties [28-

30]. These bulk materials demonstrate, using the equations of state at high pressure that, as pressure rises, the volume of the aforementioned materials decreases, as is typical for most materials [29-30]. The precise rate of compression, however, changes based on the equation of state that is applied to predict the behavior [31]. Therefore, to characterize the behavior of the material under severe pressure and temperature circumstances, we only need to know two parameters for the current investigation: the bulk modulus (B_0) and its first derivative [6-10, 32]. The ratio of the minuscule change in pressure to the corresponding fractional change in volume is known as the bulk modulus, and it expresses a material's resistance to volume change when exposed to external pressure [32-33]. Several equations of state have been provided in the section below (method of analysis) to improve the depiction of the PVT relationship for bulk materials [6-11]. In the present study we plan to investigate the compression behaviour of some bulk materials namely aluminium (Al, Z=13, Z refers to the atomic number of elements), copper (Cu, Z=29), nickel (Ni, Z=28), lead (Pb, Z=82) and zinc (Zn, Z=30) by utilizing the volume compression (V/V_0) as a function of pressure at constant temperature with the help of equations of states.

2. Methods of Analysis

In the present study, various EOS which are discussed above in the introduction, have been used to determine the compression behaviour of bulk materials namely Al, Cu, Ni, Pb and Zn by calculating the relative change in volume (V/V_0) as a function of pressure at a constant temperature [34-38]. The equations are as:

Tait equation of state is based on non-linear relation of compression with pressure for liquids [38-39]. After several modifications the new form of equation of state is introduced known as Usual Tait equation (UTE), which is in the following form and applicable for different solids.

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

Using this realistic approach, we can calculate the relative compression V/V_0 for different solids.

Also, the expression for isothermal bulk modulus $B(P)$by using relation can be written as:

$$B = B_0\frac{V}{V_0}\left\{1 + \left(\frac{B_0 + 1}{B_0}\right)P\right\}$$

$$\text{or} \qquad 1 + \left(\frac{B_0+1}{B_0}\right)P = \exp\left\{\left(1 - \frac{V}{V_0}\right)(B_0 + 1)\right\}$$

From above equations, we get

$$B(P) = B_0\frac{V}{V_0}\exp\left\{\left(1 - \frac{V}{V_0}\right)(B_0 + 1)\right\} \qquad (1)$$

The Eqn. (1) is the Tiat equation for isothermal bulk modulus.

Other equations of states, Murnaghan equation, Kholiya and Chandra equation and Shanker's equation of state are expressed as:

Murnaghan EOS [39, 40-41] is given by the relation

$$P = \frac{B_0}{B_0'}\left[\exp\left\{-B_0'\ln\left(\frac{V}{V_0}\right)\right\} - 1\right] \qquad (2)$$

Kohliya and Chandra [38, 42-43] equation of state is given the relation

$$P = \frac{B_0}{2}\left[(B_0' - 3) - 2(B_0' - 2)\left(\frac{V}{V_0}\right)^{-1} + (B_0' - 1)\left(\frac{V}{V_0}\right)^{-2}\right] \qquad (3)$$

Shanker's equation of state [44-45] is given by the equation

$$P = B_0\left[\left(1-\frac{V}{V_0}\right)+\left(B_0'+\frac{1}{2}\right)\left(1-\left(\frac{V}{V_0}\right)^2\right)\right] \quad (4)$$

3. Results of Discussion

Using isothermal equations of state, the volume compression in a variety of bulk materials, including Al, Cu, Ni, Pb, and Zn, is investigated over the pressure range of 0–16 GPa in order to confirm the suitability of the current equations of state. The thermodynamic variable such as the relative change in volume (V/V0) at high pressure has been computed in this work. Table 1 displays the input data for these metals needed to calculate the volume compression in bulk form.

Table 1: Input data used for various metals.

Compounds	$\boldsymbol{B_0}$ **(GPa)**	$\boldsymbol{B_0'}$**(GPa)**
Al	72.6	4.85
Cu	135	5.93
Ni	180.39	16.48
Pb	42.38	3.74
Zn	6.46	3.29

3.1 The compression behaviour of Aluminium (Al)

The compression behavior of Al at various pressures (in GPa) as predicted by various equations of state is displayed in Table 2. The material's volume at each pressure in relation to its original volume (V0) is indicated by the V/V0 numbers in the table. With a V/V0 value of 0.858 at 16 GPa, Tait's equation predicts that the material's volume will steadily decrease as pressure increases. A similar pattern is also predicted by the Murnaghan equation, except for 16 GPa, the V/V0 value is little larger at 0.860. At 16 GPa, the Kholiya and Chandra equation predicts a faster volume reduction with a V/V0 ratio of 0.857. With a V/V0 ratio of 0.980 at 16 GPa, the Shanker's equation of state predicts a very slight drop in volume (Fig. 1). Overall, the chart demonstrates that, as is typical for most materials, the volume of aluminum (Al) decreases as the pressure rises.

Table 2: Compression behaviour of Al predicted by various EOS.

Pressure (GPa)	**Tait Equation**	**Murnaghan Equation**	**Kholiya and Chandra Equation**	**Shankers Equation**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.974	0.974	0.974	0.997
4	0.952	0.952	0.952	0.995
6	0.932	0.932	0.932	0.992
8	0.915	0.915	0.914	0.99
10	0.899	0.899	0.898	0.988
12	0.884	0.885	0.883	0.985
14	0.87	0.872	0.869	0.983
16	0.858	0.86	0.857	0.98

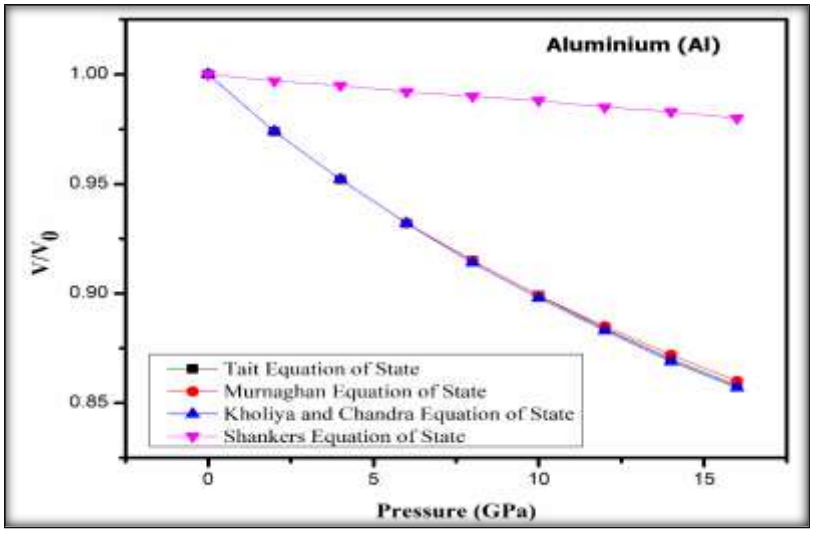

Fig 1. Volume compression with respect to pressure for Al.

3.2The compression behaviour of Copper (Cu)

The compression behavior of Cu at various pressures (in GPa) as predicted by various equations of state (Fig 2) is displayed in Table 3. According to the table, copper's volume reduces as pressure rises, which is in line with how most materials behave when compressed. At 16 GPa, the Tait equation predicts a progressive drop in volume with a V/V0 ratio of 0.914. At 16 GPa, Murnaghan's equation predicts a slightly larger V/V0 value of 0.914, which likewise indicates a progressive decrease in volume. A slightly faster volume reduction is predicted by the Kholiya and Chandra equation of state, with a V/V0 value of 0.912 at 16 GPa. At 16 GPa, the Shanker's equation of state predicts a sluggish rate of volume compression with a V/V0 value of 0.991.

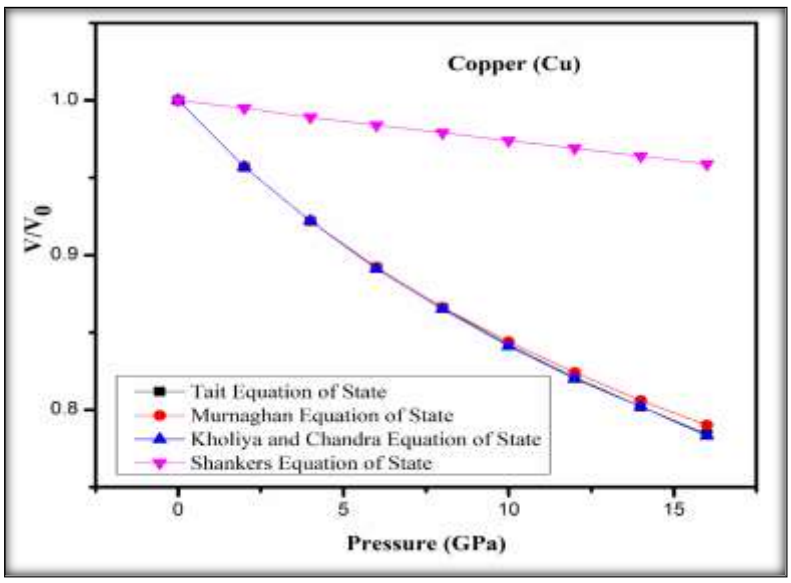

Fig 2. Volume compression with respect to pressure for Cu.

Table 3. Compression behaviour of Cu predicted by various EOS.

Pressure (GPa)	**Tait Equation**	**Murnaghan Equation**	**Kholiya and Chandra Equation**	**Shanker's Equation**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.957	0.957	0.957	0.995
4	0.922	0.922	0.922	0.989
6	0.892	0.892	0.891	0.984
8	0.866	0.866	0.865	0.979
10	0.842	0.844	0.841	0.974
12	0.821	0.824	0.82	0.969
14	0.802	0.806	0.802	0.964
16	0.784	0.79	0.783	0.959

3.3The compression behaviour of Lead (Pb)

The compression behavior of Pb at various pressures (in GPa) as predicted by various equations of state (Fig. 3) is shown in Table 4. This table shows that the volume of Pb decreases with increasing pressure, which is in line with how most materials behave when compressed.The predictions from the Tait, Murnaghan, Kholiya, and Chandra Equations are almost identical up to 8 GPa. For instance, all estimates place V/V0 = 0.866 approximately at 8 GPa and V/V0 = 0.957 approximately at 2 GPa.The volume will gradually decrease, according to Tait's equation of state, with a V/V0 ratio of 0.784 at 16 GPa.

A progressive drop in volume is also predicted by Murnaghan's equation, which similarly predicts a slightly larger V/V0 value of 0.790 at 16 GPa. A slightly faster volume reduction is predicted by the Kholiya and Chandra equation, with a V/V0 value of 0.783 at 16 GPa. With a V/V0 value of 0.959 at 16 GPa, the Shankers equation predicts a relatively gradual drop in volume.Shanker's Equation predicts less compression than the other models, particularly at lower pressures. At 2 GPa, it produces V/V0 = 0.995, indicating a slower rate of compression, but at 8 GPa, it predicts V/V0 = 0.979, which is still higher than the other equations. Even at higher pressures (10–16 GPa), Shanker's model exhibits the slowest volume decline, with V/V0 = 0.959 at 16 GPa. This implies that Shanker's Equation is more suitable for materials that can withstand compression, particularly at lower pressure ranges.

Table 4. Compression behaviour of Pb predicted by various EOS.

Pressure (GPa)	**Tait Equation**	**Murnaghan Equation**	**Kholiya and Chandra Equation**	**Shanker's Equation**
	V/V_0	**V/V_0**	**V/V_0**	**V/V_0**
0	1	1	1	1
2	0.957	0.957	0.957	0.995

4	0.922	0.922	0.922	0.989
6	0.892	0.892	0.891	0.984
8	0.866	0.866	0.865	0.979
10	0.842	0.844	0.841	0.974
12	0.821	0.824	0.82	0.969
14	0.802	0.806	0.802	0.964
16	0.784	0.79	0.783	0.959

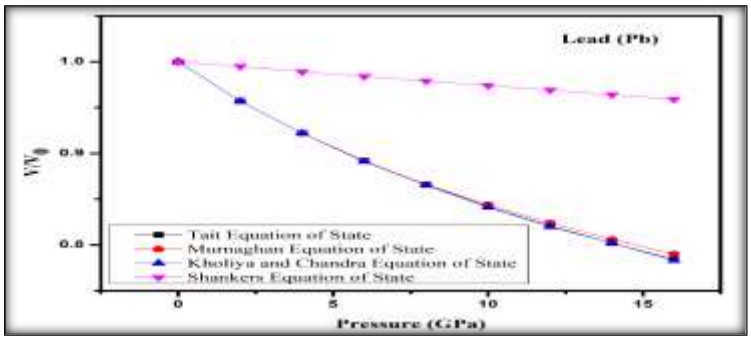

Fig 3. Volume compression with respect to pressure for Pb.

3.4The compression behaviour of Nickel (Ni)

Using several equations of states, Table 5 displays the compression behavior of Ni at different pressures. The relative volume V/V0 at each pressure point is used to tabulate the data (Fig 4). The material's volume under zero pressure is equal to its starting volume, V0, hence V/V0=1. The material is compressed when pressure is applied, which causes the volume to decrease. As pressure rises, the V/V0 value falls, suggesting that Ni is compressed when pressure is applied. Although the values derived from various equations of state varied slightly, the patterns of compression behavior are comparable. The V/V0 ratios vary from 0.947 to 0.997 at the maximum pressure of 16 GPa, which represents a compression of roughly 6.1% to 6.6% from the original volume at 0 GPa. Overall, Table 5's findings indicate that Ni is significantly compressed when pressure is applied, with the compression's magnitude growing with pressure.

Table 5**.** Compression behaviour of Ni predicted by various EOS.

Pressure (GPa)	**Tait Equation**	**Murnaghan Equation**	**Kholiya and Chandra Equation**	**Shanker's Equation**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.989	0.989	0.989	0.999
4	0.981	0.981	0.981	0.999
6	0.973	0.975	0.973	0.999
8	0.967	0.967	0.966	0.998
10	0.962	0.961	0.959	0.998
12	0.956	0.956	0.953	0.998
14	0.951	0.951	0.948	0.997
16	0.947	0.946	0.943	0.997

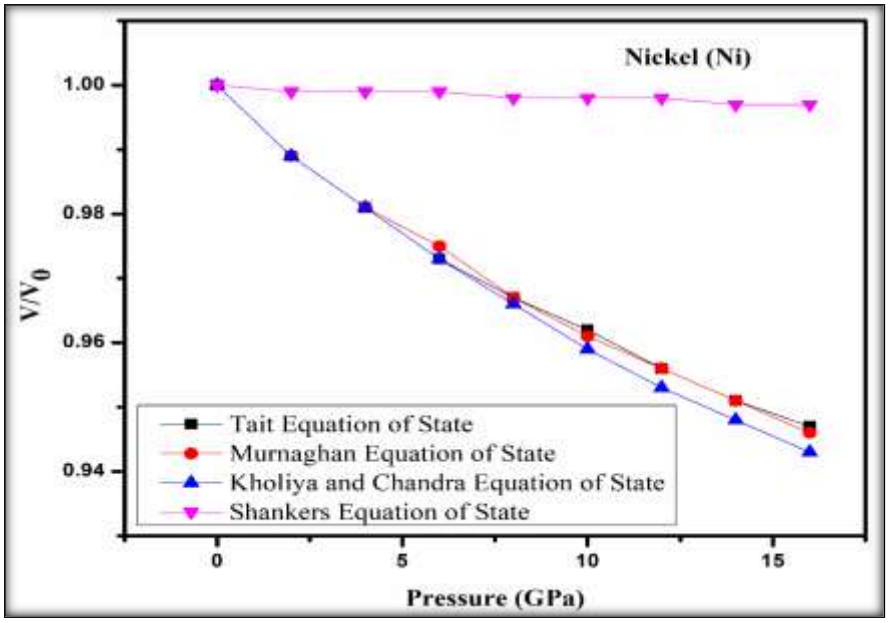

Fig 4**.** Volume compression with respect to pressure for Ni.

3.4 The compression behaviour of Zinc (Zn)

The compression behavior of zinc under different pressures, as represented by various equations of state (Fig. 5), is displayed in Table 6. As in the earlier tables, the compressibility of the material is indicated by the volume V/V0 values decreasing as the pressure rises. All of these equations of states yield results that are comparatively satisfactory overall. The variations between the various equations' anticipated values are negligible at low pressures. The discrepancies between the expected numbers, however, become increasingly noticeable as the pressure rises. Depending on the equation of state employed, the expected values of V/V0 at the maximum pressure of 14 GPa vary from 0.826 to 0.969. When compared to some of the other materials in the earlier tables, this range is quite tiny. It implies that Zn behaves rather well under high pressures and that its compression behavior is accurately described by all of the equations of state.

Table 6. Compression behaviour of Zn predicted by various EOS.

Pressure (GPa)	**Tait Equation**	**Murnaghan Equation**	**Kholiya and Chandra Equation**	**Shankers Equation**
	V/V_0	V/V_0	V/V_0	V/V_0
0	1	1	1	1
2	0.974	0.969	0.969	0.996
4	0.943	0.942	0.942	0.992
6	0.919	0.918	0.918	0.989
8	0.897	0.897	0.896	0.984
10	0.877	0.877	0.877	0.98
12	0.859	0.86	0.858	0.977
14	0.842	0.843	0.842	0.973
16	0.826	0.828	0.826	0.969

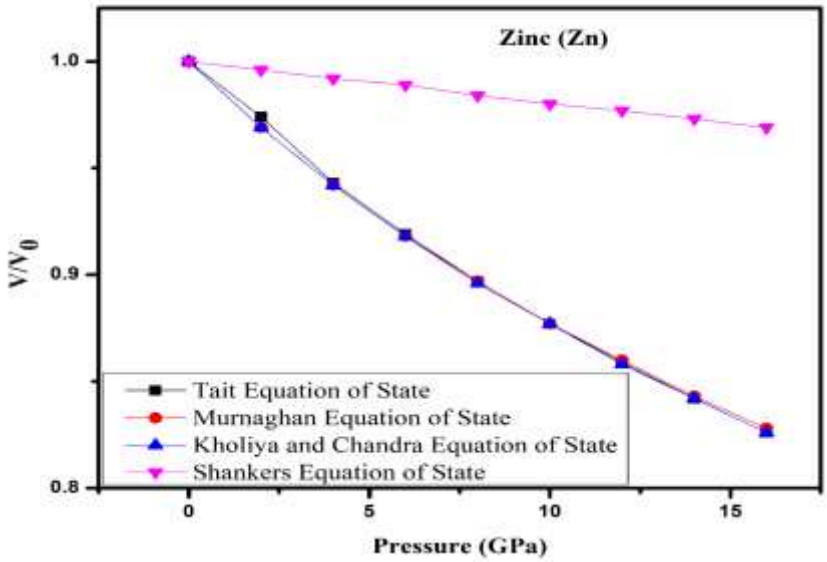

Fig 5. Volume compression with respect to pressure for Zn.

4. Conclusion:

Our study used various theoretical models or equations of state to examine the compression behavior of several bulk materials (Al, Cu, Ni, Pb, and Zn) at various pressures. The main goal of this method is to determine the relative volume (V/V_0) change with volume compression at different pressures while maintaining a constant temperature. It has been noted that the pressure and the kind of equation employed to fit the data both affect the compression behavior of the materials under study. It should be observed that when we move from nano to bulk materials, pressure causes the volume compression to drop and the bulk modulus to increase. Furthermore, the graphical depiction of the aforementioned materials shows that the compressibility of the material decreases with increasing pressure, as indicated by the value of V/V_0.Even though all bulk materials (metals) exhibit comparable patterns in their compression behavior, Shanker's equation of state demonstrated the least drop in volume compression (V/V0) among the four equations employed here.

Acknowledgement

Authors are highly thankful to the Department of Chemical Engineering and Physical science, Lovely Professional University, Phagwara,

Conflicts of Interest

Authors declare no conflicts of Interest.

Funding

The authors declare that no funds, grants, or other support were received during the preparation of this manuscript

5. References

[1] H. Nishimori, & G. Ortiz, *Oxford university press* (2011)
[2] A.K. Tyagi, & S. Banerjee (Eds.). *Materials under extreme conditions: recent trends and future prospects.* (2017)
[3] F. J. Manjón, & D. Errandonea *phys. status solidi (b).* **246** 9-31 (2009)
[4] R. Z. Valiev, R. K. Islamgaliev, & I. V. Alexandrov *Prog. Mater. Sci*. **45(2)**, 103-189 (2000).
[5] H. K. Mao, B. Chen, J. Chen, K. Li, J. F. Lin, W. Yang, & H. Zheng *MRE*. **1(1)**, 59-75 (2016)
[6] R. Kumar, & M. Kumar *IJPAP*. **51** 87-93 (2013)
[7] J. R. *RMP*. **38(4)** 669 (1966)
[8] J. D. Clayton, & J. D. *Clayton Nonlinear Elastic and Inelastic Models for Shock Compression of Crystalline Solids* **117-132** (2019)

[9] B. Jasiok, E. B. Postnikov & M. Chorążewski *PCCP*. **21(29)** 15966-15973 (2019)
[10] A.P. Srivastava, B. K. Pandey & A. K. Gupta *Introducing a Novel Method for Computing High-Compression Pressure of Carbon Nanotubes.* (2023).
[11] V. Goyal & M. *Goyal Mater. Today Proc*. (2023).
[12] J. C. Bhatt, K. Kholiya, & R. Kumar *Int. Sch. Res. Notices*. **404920** (2013).
[13] R. J. Angel, Gilio, M., Mazzucchelli, M., & Alvaro, M. (2022). Garnet EoS: a critical review and synthesis. Contributions to Mineralogy and Petrology, 177(5), 54.
[14] Wilhelmsen, Ø., Aasen, A., Skaugen, G., Aursand, P., Austegard, A., Aursand, E., ... & Hammer, M. (2017). Thermodynamic modeling with equations of state: present challenges with established methods. Industrial & Engineering Chemistry Research, 56(13), 3503-3515.
[15] Eliezer, S., Ghatak, A., & Hora, H. (2002). Fundamentals of equations of state. World Scientific.
[16] Kontogeorgis, G. M., Liang, X., Arya, A., & Tsivintzelis, I. (2020). Equations of state in three centuries. Are we closer to arriving to a single model for all applications? Chemical Engineering Science: X, 7, 100060.
[17] Ali, S. J., Swift, D. C., Wu, C. J., & Kraus, R. G. (2020). Development of uncertainty-aware equation-of-state models: Application to copper. Journal of Applied Physics, 128(18).
[18] Zharkov, V. N., & Kalinin, V. A. (1971). Equations of state for solids at high pressures and temperatures (p. 257). New York: Consultants Bureau.
[19] Tabor, D. (1991). Gases, liquids and solids: and other states of matter. Cambridge university press.
[20] Holzapfel, W. B., Hartwig, M., & Sievers, W. (2001). Equations of state for Cu, Ag, and Au for wide ranges in temperature and pressure up to 500 GPa and above. Journal of Physical and Chemical Reference Data, 30(2), 515-529.
[21] Yazdizadeh, M., Eslamimanesh, A., & Esmaeilzadeh, F. (2012). Applications of cubic equations of state for determination of the solubilities of industrial solid compounds in supercritical carbon dioxide: A comparative study. Chemical engineering science, 71, 283-299.
[22] Gross, J., & Sadowski, G. (2002). Application of the perturbed-chain SAFT equation of state to associating systems. Industrial & engineering chemistry research, 41(22), 5510-5515.
[23] Smallman, R. E., & Bishop, R. J. (2013). Metals and materials: science, processes, applications. Elsevier.
[24] Galasso, F. S. (2013). Structure and properties of inorganic solids: international series of monographs in solid state physics (Vol. 7). Elsevier.
[25] Hosono, H., & Kitano, M. (2021). Advances in materials and applications of inorganic electrides. Chemical Reviews, 121(5), 3121-3185.
[26] Sharma, P., Ganguly, M & Sahu, M. (2024). Role of transition metals in coinage metal nanoclusters for the remediation of toxic dyes in aqueous systems. R.Sc Advances. 14, 11411-11428.
[27] Raabe, D. (2023). The materials science behind sustainable metals and alloys. Chemical reviews, 123(5), 2436-2608.
[28] Hemley, R. J. (2000). Effects of high pressure on molecules. Annual Review of Physical Chemistry, 51(1), 763-800.
[29] Badding, J. V. (1998). High-pressure synthesis, characterization, and tuning of solid state materials. Annual review of materials science, 28(1), 631-658.
[30] Bai, F., Bian, K., Huang, X., Wang, Z., & Fan, H. (2019). Pressure induced nanoparticle phase behavior, property, and applications. Chemical reviews, 119(12), 7673-7717.
[31] Islam, T., Srivastava, A. K., Kaloo, M. A., & Wani, A. A. (2023). Study Of The Compression Behaviour Of Fe Cr Ti Sn And Fe Cr Ti Sb Materials Using Various Equation Of States. Elementary Education Online, 20 (6), 4961-4961.

[32] Gupta, R., & Gupta, M. (2021). Bulk modulus of second-order pressure derivative for nanomaterials. Bulletin of Materials Science, 44 (3), 218.
[33] Raju, S., Mohandas, E., & Raghunathan, V. S. (1997). The pressure derivative of bulk modulus of transition metals: An estimation using the method of model potentials and a study of the systematics. Journal of Physics and Chemistry of Solids, 58 (9), 1367-1373.
[34] Kholiya, K., & Pandey, K. (2019). High pressure compression behaviour of bulk and nanocrystalline SnO2. Journal of Taibah University for Science, 13(1), 592-596.
[35] Raju, S., Mohandas, E., & Raghunathan, V. S. (1997). The pressure derivative of bulk modulus of transition metals: An estimation using the method of model potentials and a study of the systematics. Journal of Physics and Chemistry of Solids, 58(9), 1367-1373.
[36] Kumar, M. (1995). High pressure equation of state for solids. Physica B: Condensed Matter, 212(4), 391-394.
[37] Raju, S., Mohandas, E., & Raghunathan, V. S. (1997). The pressure derivative of bulk modulus of transition metals: An estimation using the method of model potentials and a study of the systematics. Journal of Physics and Chemistry of Solids, 58(9), 1367-1373.
[38] Kholiya, K., & Chandra, J. (2014). Equation of state model for studying high-pressure compression behaviour of nanomaterials. Journal of Taibah University for Science, 8(2), 137-141.
[39] Sanchez, I. C., & Cho, J. (1995). A universal equation of state for polymer liquids. Polymer, 36(15), 2929-2939.
[40] Jasiok, B., Postnikov, E. B., & Chorążewski, M. (2019). The prediction of high-pressure volumetric properties of compressed liquids using the two states model. Physical Chemistry Chemical Physics, 21(29), 15966-15973.
[41] Macdonald, J. R. (1969). Review of some experimental and analytical equations of state. Reviews of Modern Physics, 41(2), 316.
[42] Islam, T., Srivastava, A. K., Kaloo, M. A., & Wani, A. A. (2023). Study Of The Compression Behaviour Of Fe Cr Ti Sn And Fe Cr Ti Sb Materials Using Various Equation Of States. Elementary Education Online, 20(6), 4961-4961.
[43] Kholiya, K., Chandra, J., & Verma, S. (2014). Analysis of equation of states for the suitability at high pressure: MgO as an example. The Scientific World Journal, 2014(1), 289353.
[44] Shanker, J., Kushwah, S. S., & Kumar, P. (1997). Equation of state and pressure derivatives of bulk modulus for NaCl crystal. Physica B: Condensed Matter, 239(3-4), 337-344.
[45] Kumar, M., & Kumar, M. (2007). Shanker formulation needs modification at high pressures. Journal of Physics and Chemistry of Solids, 68(4), 670-672.

Conflicts of Interest

Authors declare no conflicts of Interest.