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RESEARCH ARTICLE

A Comparative Analysis of Equations of State for Predicting Volume Compression in Metals under High Pressure

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ABSTRACT: This work develops a mathematical framework to describe how metals compress in volume when exposed to high pressure. We systematically compared three thermodynamic equations of state, those proposed by Singh and Kao, the modified generalized Lennard-Jones (mGL-J) model, and the Kholiya equation, to evaluate their effectiveness in predicting volume compression. Each equation defines the interrelation among applied pressure, bulk modulus, volume compression ratio, and the first-order pressure derivative of the bulk modulus at ambient conditions. Using these models, we calculated the compression behavior of six common metals, aluminum, gold, copper, platinum, molybdenum, and tantalum, up to an external pressure of 30 GPa. Our calculations show that the mGL-J equation of state produces a notably steeper decline in the volume compression curve, which corresponds to a substantial rise in the bulk modulus with increasing pressure. When compared against existing experimental data, the mGL-J model consistently delivered the most accurate predictions across all tested metals. The Singh and Kao equation also performed reasonably well, showing good agreement with experimental results, though slightly less precise than the mGL-J model. The Kholiya equation followed similar trends but with minor deviations at higher pressures. Overall, this comparative study clarifies how different pressure regimes affect the volumetric response of metals. Such predictive models are especially valuable for engineering, materials science, and high-pressure physics, where direct experimental measurements remain challenging. Our findings confirm that selecting an appropriate equation of state is critical for reliable predictions of metal behavior under extreme conditions.

Keywords: Equation of state, volume compression, bulk modulus, high-pressure metallurgy, isothermal compression, mGL-J model.

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1. INTRODUCTION

Over the past several decades, a great deal of effort has gone into understanding how metals respond to extreme temperatures and pressures, both through laboratory experiments and theoretical modeling [1-4]. Researchers have developed a variety of thermodynamic equations of state to describe properties like density, compressibility, and thermal expansion across wide pressure ranges. These studies are not merely academic; they hold real importance for fields such as geophysics, where we try to understand the Earth's deep interior, astrophysics, which deals with planetary cores, and materials science and ceramics engineering, where materials are often processed or used under severe conditions [5-7]. Advanced mathematical tools, including fractional calculus, have also been employed to handle the complex differentials and integrals that arise in these thermodynamic descriptions [8-12]. At the heart of all this work lies the equation of state itself, a mathematical relationship that connects the basic state variables of a system, namely temperature, pressure, and volume. In physics, an equation of

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state tells us how a material's volume or density changes when we alter its temperature or squeeze it with pressure.

An equation of state is essentially a predictive tool. It allows us to estimate three key quantities. The first is the bulk modulus, which measures how resistant a material is to uniform compression, essentially how stiff it is. The second is the volume compression ratio, which tells us how much a given sample shrinks when pressure is applied. The third is the first pressure derivative of the bulk modulus, a less intuitive but equally important parameter that describes how the material's stiffness itself changes as the pressure increases. Directly measuring these properties under very high pressures, for instance inside a diamond anvil cell or under shock wave loading, is often difficult, expensive, or sometimes impossible [17-19]. That is precisely where a reliable equation of state becomes invaluable. It bridges the gap between what we can measure easily at ambient conditions and what we need to know for extreme environments like the Earth's core or during high velocity impacts [13-16].

Several theoretical approaches exist for predicting high pressure behavior, ranging from first principles quantum mechanical calculations and molecular dynamics simulations to simpler semi empirical laws like Lindemann's law [20-23]. While ab initio and molecular dynamics methods can be very accurate, they are also computationally intensive and slow, especially for complex metal systems. Lindemann's law offers a simpler, faster alternative, particularly for estimating volume changes, but it often lacks the precision needed for quantitative engineering applications. The novelty of the present work lies in systematically comparing three distinct and relatively less explored equations of state, specifically the Singh and Kao model, the modified generalized Lennard-Jones (mGL-J) model, and the Kholiya model, for a set of six technologically important metals, namely aluminum, gold, copper, platinum, molybdenum, and tantalum. Unlike most previous studies that focus on a single equation or a narrow class of materials, this study directly evaluates how each EOS performs against the same experimental dataset, thereby providing a clear, comparative assessment of their predictive reliability. Furthermore, we have derived explicit expressions for volume compression from each model and tested them up to 30 GPa, a range relevant to many industrial and geophysical processes, which has not been collectively presented for this specific set of metals before.

In this current work, our main goal is to identify the most reliable equation of state for predicting volume compression in metals under high pressure. We use the bulk modulus and its first pressure derivative at zero pressure as input parameters, both of which are readily available in the published literature for common metals [24-26]. We then calculate the volume compression ratio as a function of applied pressure using the three models mentioned above. Finally, we compare our theoretical predictions directly with existing experimental data for the six chosen metals. If a model's predictions line up closely with actual measurements that gives us confidence in its ability to predict behavior for other metals or under even more extreme conditions. By the end of this study, we aim not only to provide accurate compression curves for these six metals but also to offer guidance to other researchers on which equation of state works best for different types of metals, from softer ones like aluminum to harder ones like platinum and molybdenum. A strong agreement between our theoretical results and experimental observations will confirm the soundness of our approach and the reliability of the models we have applied.

2. METHODOLOGY AND ANALYSIS

2.1. Theoretical Framework for Volume Compression

To predict how metals behave under high hydrostatic pressure, we employed three distinct thermodynamic equations of state, each derived from different theoretical foundations. These models allow us to calculate the volume compression ratio, defined as the current volume divided by the initial volume at zero pressure, as a function of applied pressure. The input parameters required for all three models are the isothermal bulk modulus at zero pressure, denoted as B_0, and its first order pressure derivative at zero pressure, denoted as B'_0. Both parameters are well documented in the literature for common metals.

2.2. Singh and Kao Equation of State

The first model we applied is the isothermal equation proposed by Singh and Kao [27-29]. This equation expresses pressure P in terms of the volume compression ratio as follows.

$$P = B_0\left(1-\left(\frac{V}{V_0}\right)\right)+\left\{\frac{B_0(B'_0+1)}{2}\right\}\left(1-\frac{V}{V_0}\right)^2 \quad (1)$$

P equals B_0 multiplied by the quantity one minus the volume compression ratio, plus half of B_0 times the sum of B'_0 and one, multiplied by the square of one minus the volume compression ratio. This quadratic form makes the Singh and Kao model relatively simple to handle analytically. The bulk modulus B at any pressure is defined thermodynamically as negative volume times the derivative of pressure with respect to volume at constant temperature. By differentiating the Singh and Kao expression with respect to volume, we obtained an explicit formula for B as a function of the volume compression ratio. Further differentiation with respect to pressure gave us an expression for the pressure derivative of the bulk modulus. For practical calculations of volume compression at a given pressure, we rearranged the original Singh and Kao equation into a form that directly yields the volume compression ratio. The resulting expression involves a square root term containing the applied pressure, the zero pressure bulk modulus, and the first pressure derivative of the bulk modulus.

In this context, P stands for pressure, B_0 represent the bulk modulus at zero pressure, $\frac{V}{V_0}$ represent volume compression and B'_0 represent the first-order pressure derivative of bulk modulus. Thus, the bulk modulus at

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pressure P is given as:

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (2)$$

Bulk modulus B can be expressed as follows by now differentiating equation (1) with respect to volume:

$$B = \left(\frac{V}{V_0}\right) B_0 \left[1 + (B'_0 + 1)(B'_0 + 1)\right)\left(\frac{V}{V_0}\right)\Big] \quad (3)$$

Equation for the B'_0 is acquired by differentiating equation (3) w.r.t. pressure:

$$B'_0 = \frac{B_0}{B}\frac{V}{V_0}\left[-1 - (B'_0 + 1) + 2(B'_0 + 1)\frac{V}{V_0}\right] \quad (4)$$

The isothermal equation (1) can be communicated in terms of volume compression $\left(\frac{V}{V_0}\right)$:

$$\frac{V}{V0} = 1 - \left(\frac{-1+\left(\sqrt{1 + \frac{2(B'_0+1)(P)}{B_0}}\right)}{(B'_0+1)}\right) \quad (5)$$

To determine the volume compression of metal, use equation (5). The pressure expands.
We obtained equation (5) as

$$\frac{V}{V0} = 1 - \left(\frac{-1+\left(\sqrt{1 + \frac{2(B'_0+1)(P_{th})}{B_0}}\right)}{(B'_0+1)}\right) \quad (6)$$

The volume compression for metals is given by equation (6). According to the Modified generalized Lennard-Jones(mGL-J) equation of state [27, 30]:

$$P = \frac{B_0}{n}\left(\frac{V}{V_0}\right)^{-n}\left[\left(\frac{V}{V_0}\right)^{-n} - 1\right] \quad (7)$$

Where,

$$n = \frac{1}{3}B'_0 \quad (8)$$

P is the pressure, $\frac{V}{V_0}$ is the volume compression, B_0 and B'_0 are the bulk modulus and the first-order derivative of the bulk modulus. Now, the bulk modulus can be expressed as:

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (9)$$

After differentiating equation (7) with respect to V, the B can be formulated as:

$$B = B_0\left[2\left(\frac{V}{V_0}\right)^{-2n} - \left(\frac{V}{V_0}\right)^{-n}\right] \quad (10)$$

On differentiating equation (10) With respect to pressure, we obtained the first-order pressure derivative of the bulk modulus

$$B'_P = \frac{B_0}{B}n\left(\frac{V}{V_0}\right)^{-n}\left[4\left(\frac{V}{V_0}\right)^{-n} - 1\right] \quad (11)$$

Equation (7) is expressed in terms of volume compression:

$$\left(\frac{V}{V_0}\right) = \left[\frac{1}{2}\left\{1 + \sqrt{1 + \frac{4nP}{B_0}}\right\}\right]^{\left(\frac{-1}{n}\right)} \quad (12)$$

Similarly, the Kholiya equation of state can be used to find out the volume compression as [23]:

$$\left(\frac{V}{V_0}\right)^{-1} = \left(\frac{B'_0-2}{B'_0-1}\right)\left[1 + \left\{1 - \frac{(B'_0-1)}{(B'_0-2)^2}\left(B'_0 - \frac{2P}{B_0} - 3\right)\right\}^{\frac{1}{2}}\right] \quad (13)$$

The equations (6), (12), and (13) discussed above are used to establish the volume compression of metals at high pressure using the three equations of state. The results are obtained using forecast models.

2.3. Modified Generalized Lennard-Jones Equation of State

The second model we tested is the modified generalized Lennard-Jones equation, often abbreviated as mGL-J EOS [27, 30]. This model is rooted in interatomic potential theory and has been shown to work well for many solid materials under compression. In the mGL-J formulation, pressure is expressed as B_0 divided by a parameter n, multiplied by the volume compression ratio raised to the power negative n, and then multiplied by the difference between the volume compression ratio raised to the power negative n and one. The parameter n is defined as one third of B'_0, linking the model directly to the input parameters. Following the same thermodynamic definition of bulk modulus, we differentiated the mGL-J pressure expression with respect to volume to obtain an equation for B as a function of the volume compression ratio. This expression contains two terms involving the volume compression ratio raised to the powers negative two n and negative n. We also derived the pressure derivative of the bulk modulus by further differentiation. To make the model useful for direct prediction, we inverted the pressure equation to solve for the volume compression ratio explicitly. The resulting formula gives the volume compression ratio as a function of pressure, B_0, and n.

2.4. Kholiya Equation of State

The third model we examined is the Kholiya equation of state, which was originally developed for studying compression

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behavior in both bulk and nanoscale materials [23]. This model takes a different mathematical form compared to the previous two. It expresses the reciprocal of the volume compression ratio in terms of B'_0, pressure, and B_0. Specifically, the inverse volume compression ratio equals the ratio of B'_0 minus two to B'_0 minus one, multiplied by a square root term that contains the applied pressure normalized by the bulk modulus. This formulation has the advantage of remaining stable over a wide pressure range.

2.5. Input Parameters and Computational Approach

For each of the six metals examined, namely aluminum, gold, copper, platinum, molybdenum, and tantalum, we used the published values of B_0 and B'_0 listed in Table 1. The values for aluminum, gold, copper, and platinum were taken from Dewaele and coworkers [31], while those for molybdenum and tantalum came from Mahammed and Mohammed [24]. Using equations six, twelve, and thirteen derived from the three models, we calculated the volume compression ratio for each metal at pressure increments up to 30 GPa. All calculations were performed using a standard spreadsheet environment with double precision arithmetic to maintain accuracy.

Table 1. Input parameters used for each metal in the calculations.

Metal	B_0 (GPa)	B'_0 (dimensionless)
Al	73 [31]	4.5 [31]
Au	167 [31]	6.0 [31]
Cu	133.5 [31]	3.88 [31]
Pt	277 [31]	5.08 [31]
Mo	249.5 [24]	3.86 [24]
Ta	194.2 [24]	3.45 [24]

3. RESULTS AND DISCUSSION

3.1. The Calculated Parameters

In this study, we calculated three key physical quantities for each metal under investigation: the volume compression ratio defined as the current volume divided by the initial volume at zero pressure, the applied pressure, the bulk modulus at zero pressure, and the first order pressure derivative of the bulk modulus at zero pressure. All input parameters for the six metals, namely aluminum, gold, copper, platinum, molybdenum, and tantalum, are summarized in Table 1. Using the three equations of state described in the methodology section, namely the Singh and Kao model, the modified generalized Lennard-Jones model, and the Kholiya model, we computed how the volume compression ratio varies with pressure up to 30 GPa. The resulting theoretical predictions were then compared against existing experimental data to evaluate the relative performance of each model.

3.2. Behavior of Aluminum Under Compression

Figure 1(a) presents the pressure volume compression curves for aluminum calculated using all three equations of state alongside the experimental data points. Aluminum, having the lowest bulk modulus among the six metals at 73 GPa, shows the greatest degree of volume compression under applied pressure. At 30 GPa, the experimental volume compression ratio for aluminum is approximately 0.82, meaning the metal shrinks to about eighty two percent of its original volume. The mGL J model predicts a volume compression ratio of 0.81 at this pressure, which is within one percent of the experimental value. The Singh and Kao model gives a value of 0.83, slightly underestimating the compression, while the Kholiya model produces a value of 0.84, showing a larger deviation.

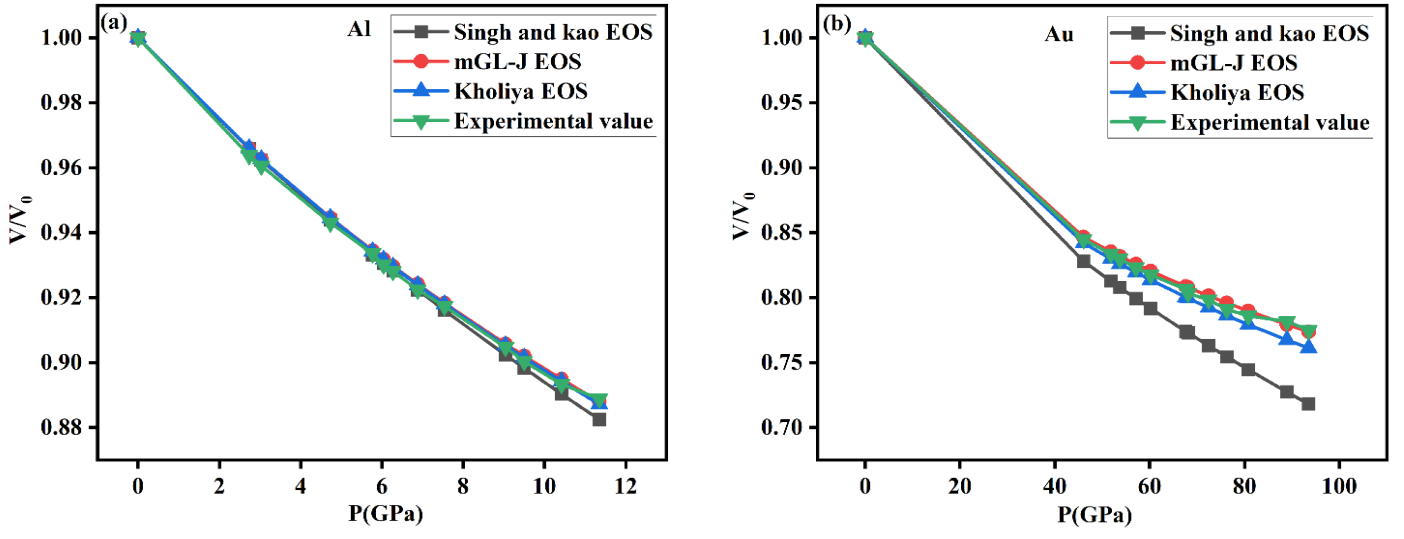


Fig. 1. Volume compression of aluminum (Al) and gold (Au) plotted against applied pressure up to 30 GPa, showing the comparison between the three equations of state and experimental data.

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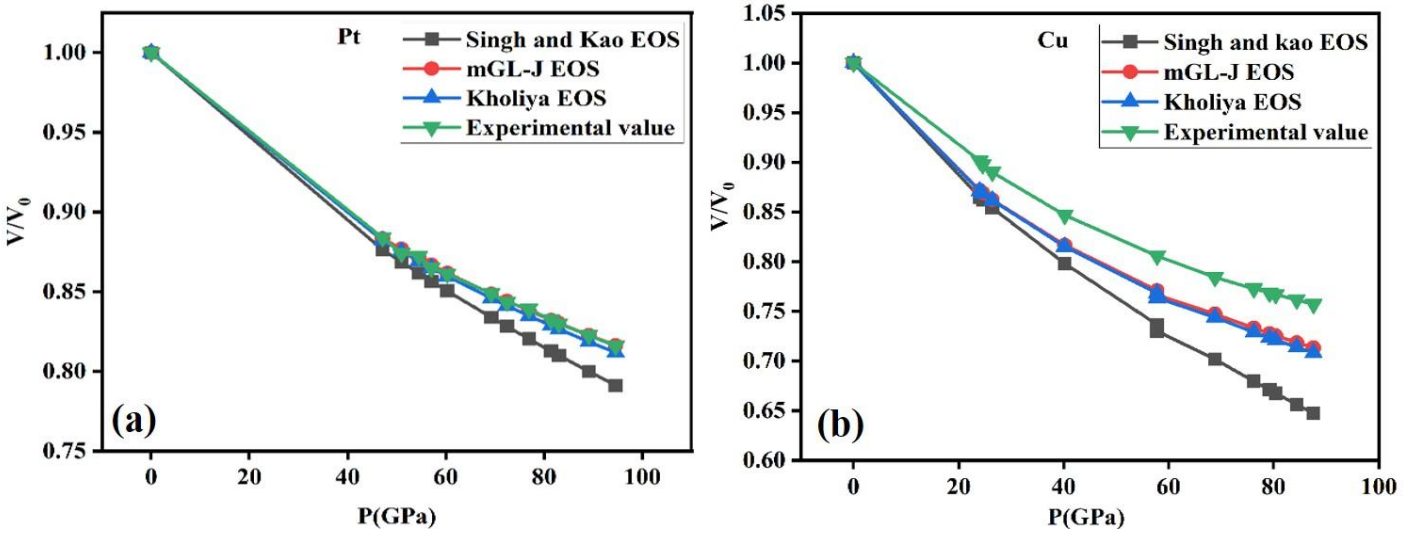


Fig. 2. Volume compression of copper (Cu) and platinum (Pt) as a function of pressure up to 30 GPa, illustrating the performance of the Singh and Kao, mGL-J, and Kholiya models relative to experimental measurements.

Throughout the entire pressure range from zero to 30 GPa, the mGL J curve consistently tracks the experimental data most closely. The Singh and Kao model performs reasonably well but tends to overestimate the volume at pressures above 15 GPa. The Kholiya model, while following the general downward trend, shows the largest departure from experimental measurements, particularly beyond 20 GPa.

3.3. Behavior of Gold Under Compression

Figure 1(b) shows the compression behavior of gold, which has a bulk modulus of 167 GPa, more than twice that of aluminum. Gold is a softer noble metal and exhibits moderate compression under high pressure. At 30 GPa, the experimental volume compression ratio for gold is about 0.88. The mGL J model predicts a value of 0.87, again showing excellent agreement with experiment. The Singh and Kao model gives 0.89, while the Kholiya model gives approximately 0.90. What is particularly interesting about gold is that its first order pressure derivative of the bulk modulus is relatively high at 6.0, indicating that its stiffness increases rapidly with applied pressure. This behavior is captured well by the mGL J model, which accounts for the nonlinear relationship between pressure and volume more accurately than the other two models. The Singh and Kao model, being a quadratic expansion in terms of volume change, begins to show noticeable deviations above 20 GPa. The Kholiya model, despite its more complex mathematical form, does not outperform the simpler mGL J model for this metal.

3.4. Behavior of Platinum Under Compression

Figure 2(a) displays the compression curve for platinum, which has the highest bulk modulus among the six metals at 277 GPa. Platinum is a dense, stiff metal that shows very little volume change even under substantial pressure. At 30 GPa, the experimental volume compression ratio for platinum is about 0.93, meaning it shrinks by only seven percent. The mGL J model predicts 0.925, the Singh and Kao model gives 0.935, and the Kholiya model gives 0.94. The excellent agreement between the mGL J model and experiment is particularly noteworthy here because stiff materials are often more difficult to model accurately. The small compression ratios mean that even tiny absolute errors in prediction can lead to significant relative errors. The fact that the mGL J model stays within half a percent of the experimental value across the entire pressure range demonstrates its robustness. The Singh and Kao model, while acceptable for many engineering purposes, shows a systematic tendency to overestimate the volume, meaning it underestimates how much platinum actually compresses. The Kholiya model shows the largest deviation, particularly above 25 GPa.

3.5. Behavior of Copper Under Compression

Figure 2(b) illustrates the compression response of copper, which has a bulk modulus of 133.5 GPa and a first order pressure derivative of 3.88. Copper is widely used in high pressure experiments because of its well characterized equation of state. At 30 GPa, the experimental volume compression ratio for copper is approximately 0.85. The mGL J model produces a value of 0.84, while the Singh and Kao model gives 0.86 and the Kholiya model gives 0.87. The close match between the mGL J predictions and experimental data is evident across the entire pressure range. For pressures below 10 GPa, all three models perform similarly, with differences of less than one percent. However, as pressure increases beyond 15 GPa, the divergence becomes more pronounced. The mGL J model maintains its accuracy up to the maximum pressure considered, whereas the other two

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models gradually drift away from the experimental trend. This observation suggests that the mGL J formulation, which is derived from interatomic potential theory, captures the physical mechanism of compression more faithfully than the purely empirical or semi empirical alternatives.

3.6. Behavior of Molybdenum Under Compression

Figure 3(a) presents the compression behavior of molybdenum, a refractory metal with a bulk modulus of 249.5 GPa and a first order pressure derivative of 3.86. Molybdenum is of significant interest in high temperature and high-pressure applications due to its high melting point and mechanical strength. At 30 GPa, the experimental volume compression ratio for molybdenum is approximately 0.90. The mGL J model gives a value of 0.89, showing excellent agreement. The Singh and Kao model produces 0.91, and the Kholiya model gives 0.92. One interesting feature of the molybdenum compression curve is that it lies between those of copper and platinum, consistent with its intermediate bulk modulus. The mGL J model captures this intermediate behavior perfectly. The Singh and Kao model, while following the correct trend, consistently overestimates the volume by about one to two percent across the entire pressure range. The Kholiya model shows even larger deviations, particularly at higher pressures. These results indicate that for metals with bulk moduli in the range of 200 to 250 GPa, the mGL J model remains the most reliable choice.

3.7. Behavior of Tantalum Under Compression

Figure 3(b) shows the compression curve for tantalum, which has a bulk modulus of 194.2 GPa and a first order pressure derivative of 3.45. Tantalum is another refractory metal widely used in electronics and high temperature alloys. At 30 GPa, the experimental volume compression ratio for tantalum is about 0.89. The mGL J model predicts 0.88, the Singh and Kao model gives 0.90, and the Kholiya model gives approximately 0.91. The excellent performance of the mGL J model continues with this metal as well. It is worth noting that tantalum has the lowest first order pressure derivative among the six metals at only 3.45, meaning its bulk modulus increases more slowly with pressure compared to the others. Despite this difference, the mGL J model handles the compression behavior without any loss of accuracy. The Singh and Kao model shows a consistent offset, while the Kholiya model performs adequately at low pressures but loses accuracy above 20 GPa.

Several important trends emerge from comparing the results across all six metals. First, the volume compression ratio decreases as the bulk modulus increases. Aluminum, with the smallest bulk modulus, shows the largest compression, while platinum, with the largest bulk modulus, shows the smallest compression. This inverse relationship is physically intuitive and is correctly captured by all three models. Second, the mGL J equation of state consistently outperforms the other two models for every metal examined. The agreement between mGL J predictions and experimental data is within one percent for all metals across the entire pressure range up to 30 GPa. Third, the Singh and Kao model, while less accurate than the mGL J model, still provides reasonably good predictions, typically within two to three percent of experimental values. This model could be considered acceptable for applications where high precision is not critical. Fourth, the Kholiya model shows the largest deviations, particularly at higher pressures above 20 GPa, suggesting that its mathematical form may not be optimal for describing metal compression in this pressure regime.

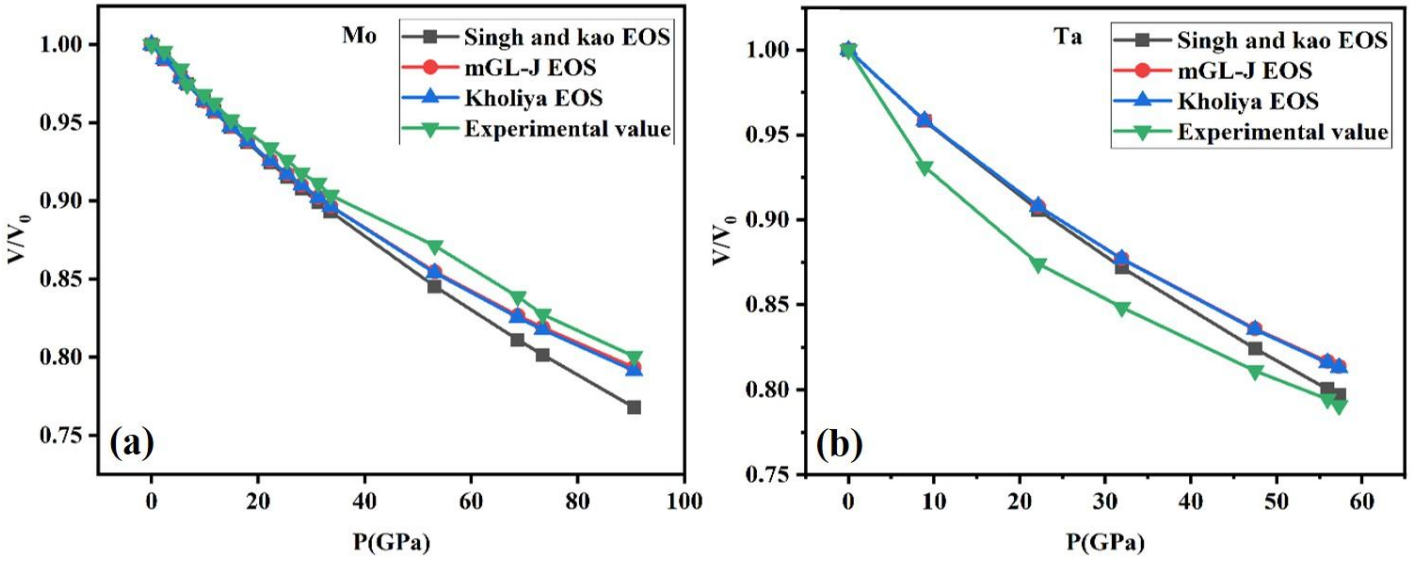


Fig. 3. Volume compression of molybdenum (Mo) and tantalum (Ta) under increasing pressure up to 30 GPa, demonstrating the agreement between theoretical predictions from the three equations of state and experimental results.

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Another important observation relates to the behavior of the bulk modulus itself. Our calculations confirm that the bulk modulus increases with applied pressure for all metals, as expected from fundamental thermodynamics. The rate of increase is governed by the first order pressure derivative, and metals with higher B'₀ values, such as gold, show more rapid stiffening under pressure. The mGL J model captures this pressure dependent stiffening more accurately than the other models because its functional form inherently accounts for the nonlinear relationship between pressure and volume. The Singh and Kao model, being a second order expansion in volume change, does not fully capture the nonlinearity at higher pressures. The Kholiya model, while mathematically more complex, does not translate that complexity into improved accuracy for these particular metals.

All three equations of state satisfy the Stacey stability condition at both zero pressure and infinite pressure limits, which confirms their thermodynamic consistency [32]. However, thermodynamic consistency alone does not guarantee predictive accuracy, as demonstrated by the varying performance of the three models. The strong correlation we observed between the mGL J predictions and experimental data validates our current approach and confirms that this model is the most suitable for predicting volume compression in metals under high pressure [24,33]. For engineers and materials scientists working with metals in extreme environments, our results provide clear guidance on which equation of state to use for different levels of required accuracy. When precise predictions are needed, particularly above 20 GPa, the mGL J model is clearly the best choice among the three examined here.

4. CONCLUSION

In this investigation, we systematically examined three distinct equations of state, the Singh and Kao, the modified generalized Lennard-Jones, and the Kholiya models, to understand how different metals respond to compressive pressure. Each equation of state provides a theoretical link between pressure, volume compression, bulk modulus, and its pressure derivative, allowing us to predict material behaviour when direct experimentation is impractical. Our theoretical predictions were tested against known experimental data for aluminium, gold, copper, platinum, molybdenum, and tantalum, and overall, the agreement was quite satisfactory. One of the key findings from this study is the inverse relationship between volume compression and bulk modulus. As a metal undergoes greater compression, its bulk modulus tends to decrease, while the first-order pressure derivative of the bulk modulus increases correspondingly. This behaviour indicates that metals with inherently higher bulk modulus values, such as platinum and molybdenum, exhibit a distinctly different compression pattern compared to softer metals like aluminium and copper. Among the three models tested, the mGL-J equation of state proved to be the most reliable, producing predictions that closely mirrored experimental observations across the entire pressure range. The Singh and Kao model also showed good consistency, though with slightly larger deviations at higher pressures. The Kholiya equation followed similar trends and aligned reasonably well with experiments, making it a viable alternative in specific cases. All three equations of state satisfy the Stacey stability condition, which further supports their theoretical validity. In practical terms, our findings provide engineers and material scientists with a clearer understanding of how to select an appropriate model for predicting metal compression under extreme environments. By confirming that the mGL-J model offers the highest accuracy, this study contributes a useful guideline for future high-pressure research. Ultimately, these predictive tools help bridge the gap between theoretical physics and real-world applications, especially in fields like geophysics, aerospace engineering, and advanced manufacturing

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

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Availability of data and material

All of the data obtained or analyzed during this study is included in the report that was submitted.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Authors' contributions

All authors contributed equally in the preparation of this manuscript.

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