Journal of Information Systems Engineering and Management
2025, 10(57s)
e-ISSN: 2468-4376
https://www.jisem-journal.com/

Research Article

Exploring the Effects of Higher Compression Orders on the Precision of the Equation of State: A Focus On HCP-Iron as A Case Study

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ARTICLE INFO

Received: 30 Dec 2024

Revised: 19 Feb 2025

Accepted: 27 Feb 2025

ABSTRACT

Our current research focuses on precisely determining the properties of hcp-iron under extreme compression. We have achieved significant strides in this area by creating a model that incorporates a minimum of eight equations of state. Our comprehensive analysis has unveiled a direct relationship between compression, pressure, and bulk modulus, offering insights into the effect of compression on the Gruneisen parameter. Additionally, we underscore the efficacy of the Srivastava-Pandey equation of state and Birch-Murnaghan in accurately characterising the properties of hcp-iron. This discovery holds promising implications for the realm of material science and engineering. We have observed that equations of state with a higher compression degree exhibit great potential in forecasting hcp-iron properties under high-pressure and compression conditions.

Keywords: Compression. Equation of state, Bulk modulus, Gruneisen parameter, hcp-Iron.

1. INTRODUCTION:

The Grüneisen parameter, a crucial thermodynamic quantity, is pivotal in unravelling the intricate connection between a material's vibrational properties and its equation of state (EOS). This research, which focuses on iron's hexagonal close-packed (hcp) phase at high pressures, is profoundly important in studying the Earth's core [1]. Hcp-Fe, believed to be the dominant phase in the core, underscores the importance of exploring the Grüneisen parameter's equation of state under extreme conditions. This exploration is a critical factor in our broader understanding of the physical properties of iron at core pressures and temperatures [2-3].

As hcp-Fe is subjected to high pressures, such as those found in the Earth's core, the behaviour of the Grüneisen parameter becomes increasingly intricate and challenging to understand. Accurately modelling the Grüneisen parameter is crucial for predicting the material's response to such conditions, which has significant implications for geophysics and planetary science. However, despite extensive studies, discrepancies remain in the values of the Grüneisen parameter derived from different experimental and theoretical approaches, raising urgent questions about the validity of the commonly used EOS formulations. This urgency underscores the pressing need for our research, which is timely and of utmost importance [4-6].

The Grüneisen parameter (γ) of hexagonal close-packed (HCP) iron is crucial for understanding Earth's core conditions. It links thermal expansion, vibrational properties, and elasticity under extreme pressure. Since HCP iron is the dominant phase in the inner core, γ helps model its thermal conductivity, seismic behaviour, and energy transport. Accurate γ values refine equations of state, improving predictions of core evolution and geodynamo function. This makes it essential for planetary science [7-8].

This study is designed to bridge these gaps by rigorously evaluating the EOS for the Grüneisen parameter of hcp-iron under high-pressure conditions. We aim to identify the most accurate and reliable formulation by comprehensively

Journal of Information Systems Engineering and Management
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comparing various models and experimental data. This will not only significantly enhance our understanding of hcp-iron's thermodynamic properties at extreme pressures but also has the potential to make a tangible and significant impact on geophysics and planetary science. By refining models of the Earth's core, our research can advance our understanding of the Earth's interior, leading to practical implications in the field. The potential impact of our work in these fields is substantial and should not be underestimated [10-15].

In our current research, we analysed a series of equations to calculate the Gruneisen parameter of hexagonal close-packed (hcp) iron under various levels of compression and pressure, with the upper limit reaching 360 GPa. Additionally, we examined the impact of higher-order compression on the Gruneisen parameter by incorporating a new third-order compression-dependent equation of state developed by Abhay et al. [16]. Furthermore, we thoroughly assessed the suitability of this equation of state in our analysis.

2. THEORETICAL MODEL:

Abhay et al. have recently developed a novel exponential equation of state broadly used as Srivastava-Pandey EOS [16-17]. This equation incorporates a third-order approximation to effectively address anharmonicity under high compression conditions. It's important to note that the accuracy of the equation significantly improves as the degree of compression increases. The equation is expressed as [18]:

$$P = K_0\left(\frac{V}{V_0}\right)^{-4/3}\left[\frac{\left\{\alpha^3(1+y+y^2+y^3)+\alpha^2(-3y^2-2y-1)+\alpha(6y+2)-6\right\}e^{\alpha y}-(\alpha^3-\alpha^2+2\alpha-6)}{\alpha^4}\right] \quad (1)$$

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

The Vinet equation of state, also known as the Universal Equation of State, describes the pressure-volume relationship of solids under high pressure. It is used in geophysics and material science to study materials under extreme conditions. At the same time, influential in modelling, accurate parameters for specific materials and conditions are required [18].

$$P = 3K_0x^{-2}(1-x)\exp\{\eta(1-x)\} \quad (2)$$

where, $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}\left(K_0^{'}-1\right)$

The Birch-Murnaghan equation of state is a widely accepted model for describing how solids behave under high pressure. Derived from finite strain theory and including higher-order terms, it provides a more accurate representation of material behaviour, making it invaluable in geophysics and material science [19-20].

$$P = \frac{3}{2}K_0[x^{-7}-x^{-5}]\left[1+\frac{3}{4}\left(K_0^{'}-4\right)\left(x^{-2}-1\right)\right] \quad (3)$$

Where $x = \left(V/V_0\right)^{1/3}$.

The Murnaghan equation of state is an essential model for understanding the compressibility of solids in geophysics and material science. For extreme conditions, more complex models like the Vinet equation may be more accurate [20].

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

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The Kholiya equation of state describes the relationship between pressure, volume, and temperature for high-pressure materials. It predicts the melting temperatures of metals and the compression behaviour of nanomaterials. The equation has been compared with others and has provided closer agreement with experimental data for certain materials, making it valuable in high-pressure physics and materials science applications [21].

$$P=\frac{K_0}{2}\left[\left(K_0^{'}-3\right)-2\left(K_0^{'}-2\right)\left(\frac{V}{V_0}\right)^{-1}+\left(K_0^{'}-1\right)\left(\frac{V}{V_0}\right)^{-2}\right] \tag{5}$$

The Usual-Tait equation of state is a mathematical model that characterises the behaviour of liquids under varying pressure conditions. Initially formulated for water, this equation has proven its versatility through extensions to a diverse range of fluids. It plays a crucial role in fields such as hydrodynamics and engineering, where precise modelling of liquid compressibility is essential for various applications, including fluid dynamics simulations and material design [22].

However, despite its utility for liquids, the Usual-Tait model is not ideally suited for exploring solids' equation of state (EOS) subjected to high-pressure environments. Several fundamental limitations hinder its application in this context. Primarily, the model was conceived for fluids, casting doubt on its effectiveness when applied to the solid state of matter. Furthermore, it falls short in providing a robust physical framework capable of addressing the intricate anharmonic effects and electronic contributions that become significant in solids under extreme compressive forces.

Moreover, the Usual-Tait equation does not accurately capture the phenomena associated with pressure-induced phase transitions—transformations that can drastically alter a material's structure and properties under pressure. Additionally, it fails to account for the nonlinear elasticity that typically manifests in solids at elevated pressures, which is critical for understanding their mechanical behaviour in such conditions. The authors of this study aim to justify the use of the Usual-Tait model by demonstrating its applicability and validity for describing the behaviour of solids, even amidst these inherent limitations.

$$P=\frac{K_0}{\left(K_0^{'}+1\right)}\left[\exp\left\{\left(K_0^{'}+1\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{6}$$

The Born-Mie equation of state (also known as the Born-Mayer equation) is a model used in thermodynamics to describe the properties of simple molecular fluids, particularly gases and liquids. It's named after Max Born and Maria Goeppert-Mayer, who developed it in the early 20th century. This equation describes the intermolecular potential energy between particles in a fluid, considering both repulsive and attractive forces between molecules [20].

$$P=\frac{3K_0}{3K_0^{'}-8}\left[\left(\frac{V}{V_0}\right)^{\frac{4}{3}-K_0^{'}}-\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\right] \tag{7}$$

The Brennan-Stacey equation of state is a model used in thermodynamics to describe the behaviour of fluids, particularly gases. It is named after its developers, R.E. Brennan and F.D. Stacey, who introduced it in 1962. This equation describes the properties of gases at high pressures and temperatures, where ideal gas behaviour breaks down. Unlike the perfect gas law, which assumes that gas particles have no volume and do not interact with each other, the Brennan-Stacey equation of state accounts for both molecular volume and intermolecular forces [23].

$$P=\frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0^{'}-5\right)}\left[\left\{\exp\left(\frac{3K_0^{'}-5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{8}$$

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where $x = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $f = \frac{3}{2}\left(K_0^{'} - 3\right)$.

Understanding the bulk modulus of a material is crucial as it helps us determine its ability to withstand changes in volume when exposed to pressure from all sides. This mechanical property is fundamental for structural solids and can be deduced by measuring the unit cell volume. To calculate the isothermal bulk modulus (K_T), we can use the following equation [18]:

$$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T \tag{9}$$

Studying the behaviour of solids under high compression is of utmost importance in various scientific fields, such as materials science and geophysics. The first-order derivative of the bulk modulus concerning pressure is a critical factor that provides valuable insights into the thermoelastic properties of solids under extreme conditions. Recent studies consistently demonstrate that this derivative decreases as pressure increases, eventually reaching a constant value. These findings offer a solid foundation for predicting the behaviour of materials under extreme conditions and have substantial implications for the development of new technologies. The formula for calculating the first-order derivative of bulk modulus for pressure at a given temperature is [18]:

$$K_T^{'} = \left(\frac{dK_T}{dP}\right)_T = -\frac{V}{K_T}\left(\frac{dK_T}{dV}\right)_T \tag{10}$$

Equations (10) and (11) allow for the calculation of the bulk modulus and the first derivative of the bulk modulus at different pressures for Srivastava-Pandey EOS, Vinet EOS, Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS, Born-Mie EOS, and Brennan-Stacey EOS.

The Gruneisen parameter (γ) plays a crucial role in thermodynamics, particularly in understanding its pressure (volume) dependence. Despite the challenges posed by the lack of a comprehensive theory and insufficient experimental data, the ongoing efforts to address these issues offer great potential for advancing our understanding of this fundamental concept. Delving deeper into exploring the Gruneisen parameter promises significant progress in thermodynamics. Furthermore, the Borton and Stacey formula has proven to effectively compute the Gruneisen parameter at high compression, offering a valuable tool for advanced studies in this area. Irvin and Stacey [25] generalised the Vashchenko-Zubarev formula [26] by accounting for non-central interatomic forces. They added a term f to the expression for the interatomic force constant and obtain the formula and the formula for Gruneisen parameter can be expressed as [27-28].

$$\gamma = \frac{\frac{K_T^{'}}{2} - \frac{1}{6} - \frac{f}{3}\left(1 - \frac{P}{3K_T}\right)}{\left(1 - \frac{4P}{3K_T}\right)} \tag{11}$$

Where f is a parameter used to fit the material's molecular structure and properties. According to Stacey's criterion, the parameter f lies between 0 and 2.5.

When the condition of the equation of state is applied, specifically at $V = V_0$, P=0, K=K_0 , K=K_0' and γ=γ_0=1.71, then the result for hcp-iron is f=2.305.

Therefore, equation (11) becomes the following for hcp-iron:

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$$\gamma = \frac{\frac{K_T^{'}}{2} - \frac{1}{6} - \frac{2.305}{3}\left(1 - \frac{P}{3K_T}\right)}{\left(1 - \frac{4P}{3K_T}\right)} \tag{12}$$

Table 1: The values of input parameters used in calculations for hcp-iron.

Parameters	Values for Hcp-Iron	References
Bulk Modulus at zero pressure K_0 (GPa)	174	[24]
The first derivative of bulk modulus at zero pressure K_0'	5.29	[24]
Gruneisen parameter at zero pressure γ_0	1.71	[25]

Table 2: The average percentage deviation in the Gruneisen parameter compared to experimental data for various equations of state.

Equation of state	Average percentage deviation
Srivastava-Pandey EOS	6.11
Vinet EOS	20.33
Birch-Murnaghan EOS	9.09
Murnaghan EOS	55.04
Kholiya EOS	25.45
Usual-Tait EOS	15.24
Born-Mie EOS	18.13
Brennan-Stacey EOS	13.57

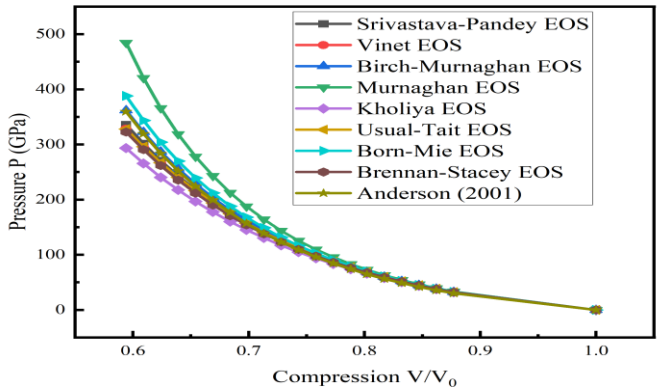

Fig. 1. Variation of pressure at different compression for hcp-Iron.

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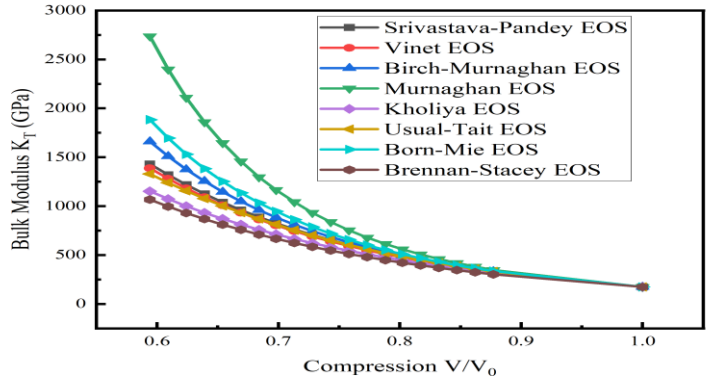

Fig. 2. Variation of bulk modulus at different compression for hcp-Iron.

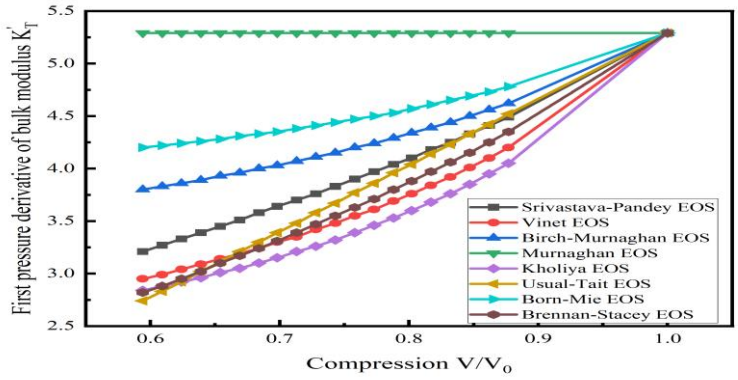

Fig. 3. Variation of first pressure derivative of bulk modulus at different compression for hcp-Iron.

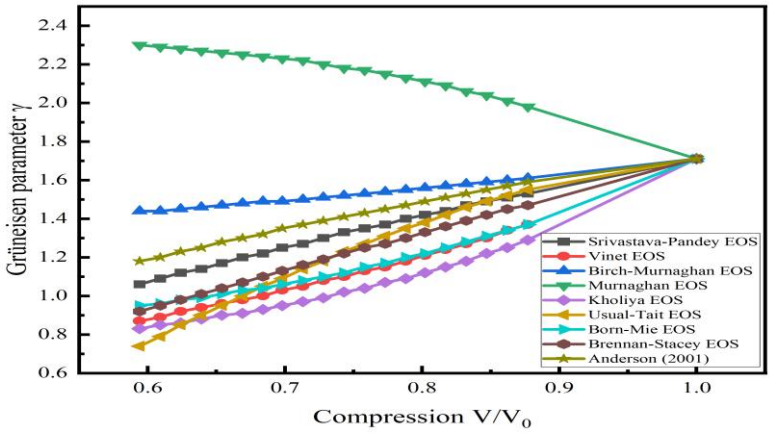

Fig. 4. Variation Grüneisen parameter at different compression for hcp-Iron.

3. RESULT AND DISCUSSION:

In our investigation of how the Grüneisen parameter of hcp-iron changes with compression, we carefully selected eight different equations of state, which are fully detailed in section 2 of our study, and the input parameters used are provided in Table 1. Equations 1 through 8 explicitly define these equations. In this study, we used equations (1)

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e-ISSN: 2468-4376
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through (8) and equations (9) and (10) to calculate the compression-dependent pressure, bulk modulus, and the first pressure derivative of the bulk modulus. We then found the parameter f to be 2.305 by applying the equation of state condition. $\left(\frac{V}{V_0}=1 \text{ and } P=0\right)$ and using the values of K_0 and K_0'. Subsequently, we calculated the compression Grüneisen parameter using equation (12). To analyse the suitability of the equation of state, we plotted the curves of compression versus pressure, compression versus bulk modulus, compression versus the first pressure derivative of bulk modulus, and compression versus Grüneisen parameter, as shown in Fig. 1-4. Additionally, to predict a suitable equation of state for calculating the Grüneisen parameter at high compression, we calculated the average percentage deviation for each equation of state listed in Table 2.

Figure 1 depicts the alignment between the Birch-Murnaghan equation of state (EOS) and the experimental data, indicating a strong correlation. Similarly, the Srivastava-Pandey EOS demonstrates results that closely resemble the experimental values. Notably, both of these third-order equations of state distinguish themselves from lower-order equations, suggesting that increasing the order of the equation of state can improve accuracy [22]. In contrast, the results obtained from other state equations show substantial deviation and lower accuracy.

Upon examination of Figure 2 and Figure 3, it is evident that as compression increases, the bulk modulus also increases, while the first pressure derivative of bulk modulus decreases with more excellent compression. Interestingly, at low compression, the results obtained from various equations of state appear pretty similar. However, at high pressure, a significant deviation is observed. Specifically, the results obtained from the Srivastava-Pandey EOS, Vinet EOS, and Usual-Tait EOS show a striking resemblance, whereas other equations of state exhibit the maximum deviation. The first pressure derivative of bulk modulus obtained by Murnaghan EOS remains constant in the derivation. Murnaghan assumed that the derivative of the bulk modulus concerning pressure is continuous. In reality, this derivative can vary with pressure, leading to inaccuracies when applying the Murnaghan EOS outside the conditions for which it was fitted.

The data depicted in Figure 4 reveals a distinct linear trend indicating a decrease in the Gruneisen parameter values with increasing pressure and compression. This trend suggests that as materials are subjected to greater external forces, their vibrational properties, as represented by the Gruneisen parameter, tend to diminish. A comparison with experimental values showcases that the Srivastava-Pandey equation of state accurately describes the system's behaviour under these conditions. While it strongly correlates with the experimental results [29], some deviation from the predicted linear trend is observed, particularly at high compression levels. This deviation is likely attributed to the onset of anharmonic effects, which become more pronounced under extreme conditions, leading to non-linear behaviour that is not accounted for in the original linear framework. These anharmonic effects alter vibrational modes, influencing the Gruneisen parameter's response to pressure and compression.

The Birch-Murnaghan equation also shows similarity to experimental values, although it exhibits slightly lower accuracy compared to the Srivastava-Pandey EOS. On the other hand, alternative equations of state display more pronounced deviations from experimental values, particularly at higher compression levels. To provide a comprehensive evaluation, we calculate the average percentage deviation against the experimental values, revealing that the Srivastava-Pandey EOS exhibits superior accuracy. At the same time, the Birch-Murnaghan equation also performs relatively well, although with reduced precision. In contrast, the average percentage deviation for the other equations of state is significantly higher, indicating substantial discrepancies from the experimental values.

The Srivastava-Pandey EOS and Birch-Murnaghan EOS are both third-order compression-dependent equations of state. However, the Srivastava-Pandey EOS sets itself apart by considering the third-order and anharmonicity of solids at high compression, which results in increased accuracy. In contrast, the Birch-Murnaghan EOS is grounded in finite strain theory, which assumes a specific strain-energy relationship. This assumption may not apply to all materials, particularly those with intricate microstructures or non-linear elastic behaviour under extreme conditions. The Srivastava-Pandey EOS is derived from the Gruneisen theory, which considers the anharmonicity of solids and presents itself as an exponential equation of state. Consequently, it can model both the non-linear and linear behaviour of solids, particularly under extreme compression.

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e-ISSN: 2468-4376
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4. CONCLUSION:

After conducting a comprehensive analysis of different state equations, it was found that the Srivastava-Pandey equation of state is remarkably effective in accurately predicting the Gruneisen parameter of hcp-Iron. Additionally, the Birch-Murnaghan equation of state has demonstrated precise predictions with minimal deviation, particularly at high compression. Conversely, other equations of state have exhibited significant deviations from experimental values. It is important to note that the observed variations in results depend on the order of compression and the fundamental assumptions made during derivation. Consequently, it can be concluded that higher-order equations of state are more suitable for accurately predicting compression-dependent properties of solids, especially at high compression levels.

5. LIMITATION:

The Vashchenko-Zubarev formula for the Grüneisen parameter (γ) assumes a simple relationship between γ and volume but has several limitations. It is empirical, lacking a fundamental derivation, and applies mainly to simple metals, failing for complex structures. The assumption of a constant volume exponent (f) makes it inaccurate for materials undergoing phase transitions. It also ignores temperature dependence, making it unreliable at high temperatures. Additionally, experimental data deviate significantly from this model at extreme pressures, such as in Earth's core. Thus, while useful for rough approximations, it lacks accuracy for extreme conditions and complex materials.

Ethical Approval:

The authors confirm that the manuscript is their original work and has not been published anywhere else before.

Competing interests:

The authors of this paper declare that they have no known financial interests or personal relationships that could have potentially influenced the work presented in this report.

Author's Contribution:

All the authors contributed equally to this manuscript. Abhay P. Srivastava made the original draft, and Anod Kumar Singh, Reetesh Srivastava, and Harish Chandra Srivastava provided guidance and calculation tools.

Funding:

The authors state that they do not have any funding agency available.

Availability of data and Materials:

The information used to support the study's conclusions is cited in the references and is publicly accessible.

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