JOURNAL OF DYNAMICS AND CONTROL

VOLUME 8 ISSUE 9

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Abstract: *In our research, we studied how the thermoelastic properties of ε-Fe change under compression. This included looking at the bulk modulus, pressure derivative of bulk modulus, thermal expansivity, Grüneisen parameter, and Debye temperature. We used different equations to determine the Debye temperature, including the Grüneisen parameter-based and Debye models. Our analysis led us to conclude that the Debye model is better than the modified Grüneisen parameter-based model proposed by Kumari and Dass for predicting the compression-dependent Debye temperature. Additionally, we found that a new parameter is needed to calculate the Grüneisen parameter for hcp-iron, which is used to calculate the Grüneisen parameter and falls below the Stacey criterion. Our study discovered that the Birh-Murnaghan, Srivastava-Pandey, and Shanker equations of state are more accurate for predicting the thermoelastic properties of hcp-iron under higher-order compression.*

Keywords: *Equation of state, Bulk modulus, Debye Temperature, Thermal Expansivity, Gruneisen Parameter.*

1. Introduction

The isothermal equation of state, a cornerstone in physics, provides invaluable insights into the relationship between pressure, volume, and temperature for substances. Its practical applications span various scientific fields, from physics and chemistry to earth sciences.[1], [2], [3]. Understanding and applying this equation is an academic exercise and a key to unlocking profound discoveries and innovative solutions in materials science. Researchers have employed multiple methods, including first principles, density functional theory (DFT), and ab initio pseudopotential calculations, to predict the equation of state accurately. To streamline the process, scientists are exploring simplified models to develop a semi-empirical form of the equation of state for solids, promising accurate predictions with minimal input parameters. This approach can provide valuable insights into the high-pressure behaviors of materials using experimental data, underscoring the equation of state's relevance and practicality in materials science.[4], [5], [6], [7].

The equation of state for iron's solid and liquid phases has been successfully determined, uncovering important elastic properties that have implications for diverse materials. These insights into the interactions between magnetic and electronic subsystems could lead to potential applications in various fields, inspiring further research and innovation.[8], [9]. The meticulous research and optimization of physical properties critical for understanding iron's behavior under high pressure have driven significant progress in materials science. These achievements open possibilities for developing new materials with unique and valuable properties, marking an essential step in our understanding of materials science. This breakthrough is not just a scientific milestone but a potential game-changer for materials science, as it helps us gain a deeper understanding of the properties of iron and opens the door to creating new materials with predictable and optimized properties. The far-reaching impact of this work is a testament to its potential to revolutionize materials science and numerous other research areas that rely on iron properties.[10], [11], [12], [13].

Iron is essential to the Earth's core, and understanding its relationship between pressure, volume, temperature, and thermodynamic properties is crucial. Studying materials at high temperatures and pressures is essential in condensed matter physics and the earth sciences. It provides valuable insights into how materials behave under extreme conditions and helps develop new materials for various applications. Therefore, ongoing exploration of the isothermal equation of state is crucial for advancing

scientific knowledge and finding new applications for different materials. The isothermal equation of state is a fundamental concept in physics that establishes the relationship between a substance's pressure, volume, and temperature at a constant temperature. Scientists have achieved a significant breakthrough by defining the equation of state for both solid and liquid phases of iron.[14], [15], [16], [17]. This was possible by optimizing various physical properties such as heat capacity, bulk modulus, first-order derivative of bulk modulus, thermal expansivity, Debye temperature, and Gruneisen parameter.[18], [19], [20].

The recent breakthrough in understanding the properties of iron will help us design experiments to study the effects of different conditions on iron behavior. By establishing the equation of state for iron, we can also anticipate and enhance the properties of new materials. This advancement is a significant step forward in materials science, with far-reaching impacts on various research fields dependent on iron properties. Iron is crucial to the Earth's core, so understanding its thermodynamic properties is essential. Furthermore, characterizing materials under high temperatures and pressure is vital for condensed matter physics and earth sciences. Such research provides valuable insights into materials' behavior under extreme conditions and helps create new materials with diverse properties for various applications. Therefore, continuous exploration of the isothermal equation of state is vital in advancing scientific knowledge and discovering new applications for different materials.[19], [21], [22], [23], [24]. When modeling the state of the Earth's interior, it is essential to have a comprehensive understanding of thermal expansion under high temperatures and pressures. Thermal expansivity is a critical factor in the equation of state describing many crucial properties of solids. Gruneisen's rules can relate thermal expansivity to another thermodynamic parameter. To calculate the volume-dependent thermal expansion coefficient, we take the product of the thermal expansion coefficient at a particular volume V and the bulk modulus at the same volume V. The bulk modulus measures a material's ability to withstand compression and remains constant at a specific volume. On the other hand, the thermal expansion coefficient measures how a material's volume changes with temperature and can be influenced by factors such as density, temperature, and pressure.[21], [25], [26], [27].

It is crucial to understand thermal expansion at high temperatures and pressures when modeling the equation of the state of the Earth's interior. The volume-dependent thermal expansion coefficient can be calculated by taking the product of the thermal expansion coefficient and the bulk modulus at a specific volume, which are critical factors in describing the properties of solids. The mechanical properties of solids play a fundamental role in structural engineering and materials science. One key parameter to define these properties is the isothermal bulk modulus. This value can be calculated by measuring the unit cell volume of a solid. It is essential in fields such as geophysics, where the behavior of solids under high compression is of great interest.[28], [29], [30], [31].

The bulk modulus is defined as the rate of pressure change concerning volume. It determines the ability of a material to resist changes in volume when subjected to external pressure. In other words, it is a measure of a material's compressibility. The isothermal bulk modulus is calculated at a constant temperature and provides information about the material's thermal behavior. To determine the isothermal bulk modulus, we can use the equation relating the bulk modulus to the unit cell volume. The first-order derivative of the bulk modulus concerning pressure is a critical factor that provides crucial insights into the behavior of materials under compression[32], [33], [34]. It measures the material's stiffness and can be used to predict the material's response to changes in pressure. Understanding the behavior of solids under high compression is an essential area of research in materials science, geology, and planetary science. Mastering the mechanical properties of materials can help us design more robust and durable structures and gain insights into their behavior in extreme conditions, such as those found deep within the Earth's crust[35], [36], [37].

The Debye temperature is an important parameter used in studying the thermoelastic behavior of solids. It is a characteristic temperature of a solid defined within the Debye model's framework for the specific

heat of solids. The Debye model assumes that the vibrations of atoms in a solid can be treated as waves and that these waves have a range of frequencies. The Debye temperature is the temperature at which the maximum frequency of these waves is reached. At high pressure, the Debye temperature becomes compression-dependent[38], [39], [40]. This means that the Debye temperature changes as the pressure on the solid changes, and this change must be known to study the thermoelastic behavior of solids accurately. Knowledge of compression-dependent Debye temperature is also helpful in other areas of materials science, such as studying phase transitions and calculating thermal conductivity.

In this article, we calculated the compression-dependent pressure, bulk modulus, first-order pressure derivative of bulk modulus, thermal expansivity, and Debye temperature of ε-Fe using the equation of states. We also proposed a correction term in the formulation of Debye temperature by using the boundary condition of the equation of state. We found that without the correction term, the results obtained by EOS deviated significantly from experimental data. However, after incorporating the correction term, the results obtained by the formula agree with experimental values.[41], [42], [43].

2. Method of Analysis

2.1. Equation of states

We have examined nine equations of state: Srivastava-Pandey EOS, Shanker EOS, Vinet EOS, Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS, Born-Mie EOS, and Brennan-Stacey EOS. This analysis aims to gain a deeper understanding of the thermal properties of ε-Fe. This will provide valuable insights into how ε-Fe behaves under different compression ranges, ultimately contributing to advancements in the field.

(1) Srivastava-Pandey EOS:

The Srivastava-Pandey equation of state (EOS) is a new exponential equation of state based on a third-order approximation of compression. It is derived from the principles of Grüneisen theory for solids, considering the anharmonic effects at high compression, and is expressed as [44,45]:

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

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

The Shanker equation of state (EOS) is a model used to describe the behavior of solids under high pressure, particularly nanomaterials. It is derived using the Grüneisen theory of thermal expansion and is particularly useful for high-pressure physics. The Shanker EOS incorporates principles from the Grüneisen theory, which relates to thermal properties and their changes under pressure. In some contexts, the Shanker EOS is modified to include higher order terms, resulting in the Higher Order Shanker (HOS) EOS, which improves its accuracy for specific materials [46].

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0^{'}-8\right)}\left[\left\{\left(1-\frac{1}{t}+\frac{2}{t^2}\right)\left(\exp ty-1\right)\right\}+\left\{y\left(1+y-\frac{2}{t}\right)\exp ty\right\}\right] \quad (2)$$

Where $y = 1 - \frac{V}{V_0}$ and $t = K_0^{'} - \frac{8}{3}$

(3) Vinet EOS:

The Vinet equation of state, also known as the Universal Equation of State, is a phenomenological model used to describe the pressure-volume relationship of solids, particularly under high pressure. It is instrumental in geophysics and material science for studying the behavior of materials under extreme conditions. The Vinet equation is derived from the material's interatomic potential and compressibility assumptions.

The Vinet equation of state is a powerful tool for modeling the pressure-volume relationship of materials under high pressure. Based on an interatomic potential, its universal form accurately fits experimental data, making it valuable in geophysics and material science. However, its empirical nature and reliance on accurate parameters are important considerations when applying it to specific materials and conditions [44,45].

$$P = 3K_0 x^{-2}(1-x)\exp\{\eta(1-x)\} \tag{3}$$

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

(4) Birch-Murnaghan EOS:

The Birch-Murnaghan equation of state is a robust and widely accepted model for describing the compressibility of solids under high pressure. Its derivation from finite strain theory and inclusion of higher-order terms gives a more accurate representation of material behavior, making it invaluable in geophysics and material science [44,45].

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

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

(5) Murnaghan EOS:

The Murnaghan equation of state is a foundational model for understanding the compressibility of solids. It is instrumental in geophysics and material science. Its simplicity makes it a practical choice, although more complex models like the Vinet equation may improve accuracy for extreme conditions [44,45].

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

(6) Kholiya EOS:

The Kholiya equation of state describes the relationship between pressure, volume, and temperature for various high-pressure materials. This equation is handy in predicting metals' melting temperatures and nanomaterials' compression behavior. The Kholiya equation has been compared with other state equations, such as the Murnaghan and Usual-Tait equations. It has been shown to provide closer

agreement with experimental data for certain materials, especially those where the bulk modulus decreases continuously with pressure. This makes it valuable in high-pressure physics and material science applications [44.45].

$$P = \frac{K_0}{2}\left[\left(K_0^{'}-3\right)-2\left(K_0^{'}-2\right)\left(\frac{V}{V_0}\right)^{-1}+\left(K_0^{'}-1\right)\left(\frac{V}{V_0}\right)^{-2}\right] \tag{6}$$

(7) Usual-Tait EOS:

The Usual-Tait equation of state is primarily used to describe the behavior of liquids under pressure. It was initially developed to model the compressibility of water and has since been applied to other fluids. The Tait equation is handy in hydrodynamics and engineering applications where accurate modeling of liquid compressibility is required [46].

$$P = \frac{K_0}{\left(K_0^{'}+1\right)}\left[\exp\left\{\left(K_0^{'}+1\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{7}$$

(8) Born-Mie EOS:

The Born-Mie equation of state, sometimes referred to 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. The Born-Mie equation of state describes the intermolecular potential energy between particles in a fluid. It considers both the repulsive and attractive forces between molecules [44,45].

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

(9) Brennan-Stacey EOS:

The Brennan-Stacey equation of state is a model used in thermodynamics to describe the behavior 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 behavior 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[44].

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0^{'}-5\right)}\left[\left\{\exp\left(\frac{3K_0^{'}-5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{9}$$

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

2.2. Isothermal Bulk Modulus and its Derivatives:

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 [45-47]:

$$K_T = -V\left(\frac{\partial P}{\partial V}\right)_T \tag{10}$$

Mastering the behavior of solids at high compression is essential in numerous fields, including materials science and geophysics. The first-order derivative of the bulk modulus concerning pressure is a critical factor that provides crucial insights into the thermoelastic properties of solids at extreme conditions. Recent studies have consistently revealed that $\frac{dK_T}{dP}$ It decreases with increasing pressure and eventually stabilizes at a constant value. These findings provide a solid foundation for predicting the behavior of materials under extreme conditions and have significant implications for the development of new technologies. To calculate the first-order derivative of bulk modulus for pressure at a given temperature, the following formula can be used:

$$K_T^{'} = \left(\frac{dK_T}{dP}\right)_T = -\frac{V}{B_T}\left(\frac{dK_T}{dV}\right)_T \tag{11}$$

Equation (10) allows for calculating the bulk modulus for Srivastava-Pandey EOS, Shanker EOS, Vinet EOS, Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS, Born-Mie EOS, and Brennan-Stacey EOS.

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-1/3}\left(1+z+z^2+z^3\right)\exp\left(\alpha z\right)+\frac{4}{3}P \tag{12}$$

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-1/3}\left(1+y+y^2\right)\exp\left(\beta y\right)+\frac{4}{3}P \tag{13}$$

$$K_T = K_0 x^{-2}\left[1+\left\{\left(1+\eta x\right)\left(1-x\right)\right\}\right]e^{\eta(1-x)} \tag{14}$$

$$K_T = \frac{K_0}{2}\left[7x^{-7}-5x^{-5}\right]+\frac{3}{8}K_0\left(K_0^{'}-4\right)\left(9x^{-9}-14x^{-7}+5x^{-5}\right) \tag{15}$$

$$K_T = K_0\left(\frac{V}{V_0}\right)^{-K_0^{'}} \tag{16}$$

$$K_T = K_0\left(K_0^{'}-2\right)\left(\frac{V}{V_0}\right)^{-1}\left[\left(\frac{K_0^{'}-1}{K_0^{'}-2}\right)\left(\frac{V}{V_0}\right)^{-1}-1\right] \tag{17}$$

$$K_T = K_0\left(\frac{V}{V_0}\right)\exp\left\{\left(K_0^{'}+1\right)\left(1-\frac{V}{V_0}\right)\right\} \tag{18}$$

$$K_T = \frac{3K_0}{3K_0^{'}-8}\left[\left(K_0^{'}-\frac{4}{3}\right)\left(\frac{V}{V_0}\right)^{\frac{4}{3}-K_0^{'}} - \frac{4}{3}\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\right] \tag{19}$$

$$K_T = \frac{4}{3}P + K_0\left(\frac{V}{V_0}\right)^{-\frac{1}{3}} \exp\left\{\left(K_0^{'}-\frac{5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\} \tag{20}$$

Equation (11) gives the first-order derivative of bulk modulus for the Srivastava-Pandey EOS, Shanker EOS, Vinet EOS, Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS, Born-Mie EOS, and Brennan-Stacey EOS.

$$K_T^{'} = \left(1-\frac{4P}{3K_T}\right)\left(\frac{1}{3}+\frac{V}{V_0}\left\{\alpha+\frac{\left(1+2z+3z^2\right)}{(1+z+z^2+z^3)}\right\}\right)+\frac{4}{3} \tag{21}$$

$$K_T^{'} = \left(1-\frac{4P}{3K_T}\right)\left(\frac{1}{3}+\frac{V}{V_0}\left\{\beta+\frac{(1+2y)}{(1+y+y^2)}\right\}\right)+\frac{4}{3} \tag{22}$$

$$K_T^{'} = \frac{1}{3}\left[2+\eta x+\frac{x(1-\eta)+2\eta x^2}{1+(\eta x+1)(1-x)}\right] \tag{23}$$

$$K_T^{'} = \frac{K_0}{8K_T}\left[\left(K_0^{'}-4\right)\left(81x^{-9}-98x^{-7}+25x^{-5}\right)+\frac{4}{9}\left(49x^{-7}-25x^{-5}\right)\right] \tag{24}$$

$$K'_T = \frac{K_0K_0^{'}}{K_T}\left(\frac{V}{V_0}\right)^{-K_0^{'}} \tag{25}$$

$$K_T^{'} = \frac{\left(K_0^{'}-2\right)\left(\frac{V}{V_0}\right)-2\left(K_0^{'}-1\right)}{\left(K_0^{'}-2\right)\left(\frac{V}{V_0}\right)-\left(K_0^{'}-1\right)} \tag{26}$$

$$K_T^{'} = \left(K_0^{'}+1\right)\left(\frac{V}{V_0}\right)-1 \tag{27}$$

$$K'_T = \frac{3K_0}{K_T(3K_0^{'}-8)}\left[\left(K_0^{'}-\frac{4}{3}\right)^2\left(\frac{V}{V_0}\right)^{\frac{4}{3}-K_0^{'}} - \frac{16}{9}\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}\right] \tag{28}$$

$$K_T^{'} = \frac{16}{9}\frac{P}{K_T}+\left(1-\frac{4}{3}\frac{P}{K_T}\right)\left[\left\{\left(K_0^{'}-\frac{5}{3}\right)\left(\frac{V}{V_0}\right)\right\}+\frac{5}{3}\right] \tag{29}$$

2.3. 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 behavior of materials under varying temperature and pressure conditions and open new pathways to advances in material science [48].

$$\alpha K_T = \text{Constant} \tag{30}$$

Shanker and Kumar show that.

$$\alpha K_T = \alpha_0 K_0 \tag{31}$$

$$\alpha = \alpha_0 \left(\frac{K_0}{K_T} \right) \tag{32}$$

2.4. Pressure (Volume) dependence of Gruneisen parameter:

The Gruneisen parameter (γ) is a significant aspect of thermodynamics, and exploring its pressure (volume) dependence presents an exciting opportunity for theoretical and experimental advancements. Although there's a lack of a proper theory and insufficient experimental data, ongoing efforts to address these issues hold promise for advancing our understanding of this fundamental concept. Overall, by continuing to investigate the Gruneisen parameter, we will likely make significant progress in thermodynamics [49].

The Borton and Stacey formula can compute the Gruneisen parameter accurately at high compression.

$$\gamma = \frac{\frac{K_T^{'}}{2} - \frac{1}{6} - \frac{f}{3}\left(1 - \frac{P}{3K_T}\right)}{\left(1 - \frac{4P}{3K_T}\right)} \tag{33}$$

Here, f Is a fitting parameter that depends on the material's molecular structure and properties. For ε-Fe, the value will be 2.305 between Stacey's criterion 0 and 2.5.

2.5. Compression-dependent Debye temperature by Gruneisen parameter-based model:

The Gruneisen parameter in terms of Debye temperature θ_d Is given by the relation as [49]:

$$\gamma = -\left(\frac{\partial \ln \theta_d}{\partial \ln V} \right)_T \tag{34}$$

Equation (34) can also be written as

$$\gamma = K_T \left(\frac{\partial \ln \theta_d}{\partial P} \right)_T \tag{35}$$

Kumari and Dass presented the following linear relation for the pressure dependence of γ as:

$$\gamma = \gamma_0 - \lambda P \tag{36}$$

where λ is a parameter assumed to remain constant with changes in pressure. With the help of equations (35) and (36), Kumar and Dass [46] obtained the relation for the pressure dependence of Debye temperature (θ_d) as follows:

$$\ln \frac{\theta_d}{\theta_0} = -\frac{\lambda P}{K_T^{'}} + \chi \ln \left[1 + \frac{K_T^{'} P}{K_0} \right] \tag{37}$$

and

$$\chi = \frac{1}{K_T^{'}}\left[\gamma_0 + \frac{\lambda K_o}{K_T^{'}}\right] \tag{38}$$

Zheng-Hua Fang [45] proposes a new expression for the pressure dependence of the Gruneisen parameter. γ by assuming that the second-order Gruneisen parameter q is independent of pressure. This relationship is written as[45]:

$$\gamma = \gamma_0\left(1+\frac{K_T^{'}P}{K_0}\right)^{-\frac{q}{K_T^{'}}} \tag{39}$$

The knowledge of the isothermal bulk modulus K_T with pressure is needed for the derivation of the relation for the pressure dependence of θ_d. The isothermal bulk modulus varies linearly with pressure as:

$$K_T = K_0 + K_T^{'}P \tag{40}$$

Substituting equations (39) and (40) into (35), we get:

$$\frac{\partial \ln\theta_d}{\partial P} = \gamma_0 K_0^{\,q/K_t^{'}}\left(K_0 + K_0^{'}P\right)^{-\left(1+\frac{q}{K_T^{'}}\right)} \tag{41}$$

Integrating equation (41), we get the following relation of the Debye temperature. θ_d:

$$\ln\frac{\theta_d}{\theta} = \frac{\gamma_0}{q}\left[1-\left(1+\frac{K_T^{'}P}{K_0}\right)^{-q/K_T^{'}}\right] \tag{42}$$

Expanding the second term of right-hand side, then equation (42) can be written as:

$$\ln\frac{\theta_d}{\theta} = \frac{\gamma_0}{q}\left[1-\left(1-\frac{q}{K_T^{'}}\frac{K_T^{'}P}{K_0}\right)+.....\right] \tag{43}$$

At low pressure, equation (43) can be written as:

$$\ln\frac{\theta_d}{\theta} = \frac{\gamma_0 P}{K_0} \tag{44}$$

$$\frac{\theta_d}{\theta} = \exp\left(\frac{\gamma_0 P}{K_0}\right) \tag{45}$$

Expanding the right-hand side of equation (45) and neglecting the higher term then, we get an expression for pressure-dependent Debye temperature as:

$$\theta_d = \theta_0\left(1+\frac{\gamma_0 P}{K_0}\right) \tag{46}$$

Equation (46) calculates the pressure-dependent Debye temperature of solids.

2.6. Compression-dependent Debye temperature by Deby Model

Debye temperature is the characteristic of each substance appearing in Debye's theory of specific heats and given by

$$\theta_d = \frac{\hbar \omega_d}{k_B} \tag{47}$$

Where θ_d represent Debye temperature at atmospheric pressure and k_b represent Boltzmann constant. The Debye model offers a valuable perspective, treating a solid as an elastic continuum characterized by diverse frequencies. This model directly links the number of vibration modes to the system's degrees of freedom, providing a comprehensive understanding of the system's behavior. Furthermore, it highlights the significant impact of vibrational frequencies, which are intricately linked to the equilibrium position and susceptible to pressure changes due to variations in compression. Notably, the Debye temperature is sensitively tied to different compression levels through compression-dependent Gruneisen parameters, emphasizing the interconnected nature of these variables within the system [47].

$$\theta_d(P) = \theta_0 \left(\frac{V}{V_0} \right)^{-\gamma} \tag{48}$$

Table 1. The values of the input parameter:

Element	Bulk Modulus at zero pressure K_0 (GPa)	Pressure derivative of bulk modulus at zero pressure K_0'	Gruneisen parameter at zero pressure γ_0	Thermal expansion coefficient at zero pressure $\alpha_0 \times 10^{-5} K^{-1}$	Debye temperature at zero pressure θ_0 (K)
ε-Fe	174	5.29	1.71	7.83	422

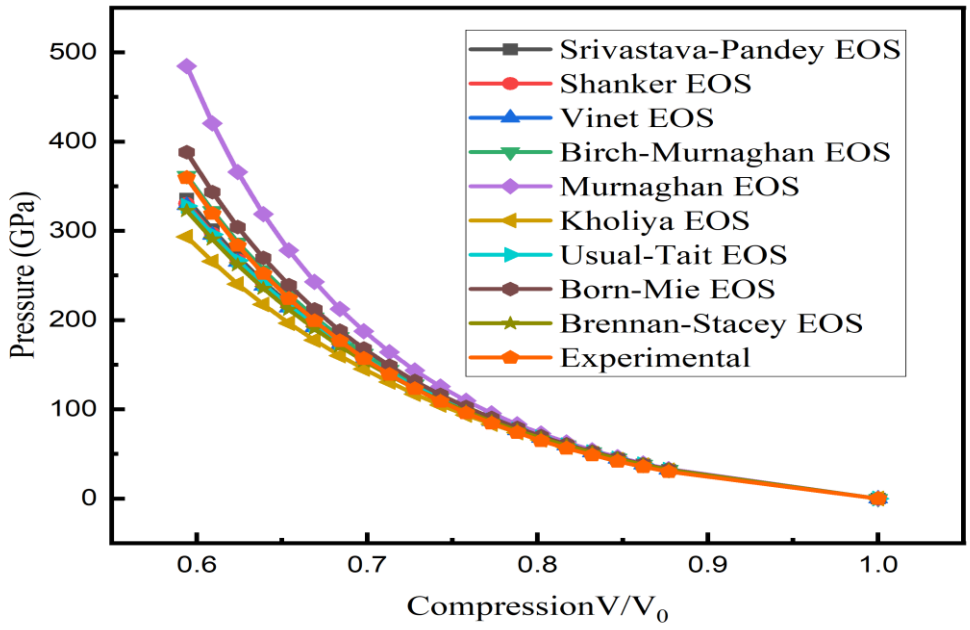

Fig. 1. Variation of pressure with different compression for ε-Fe.

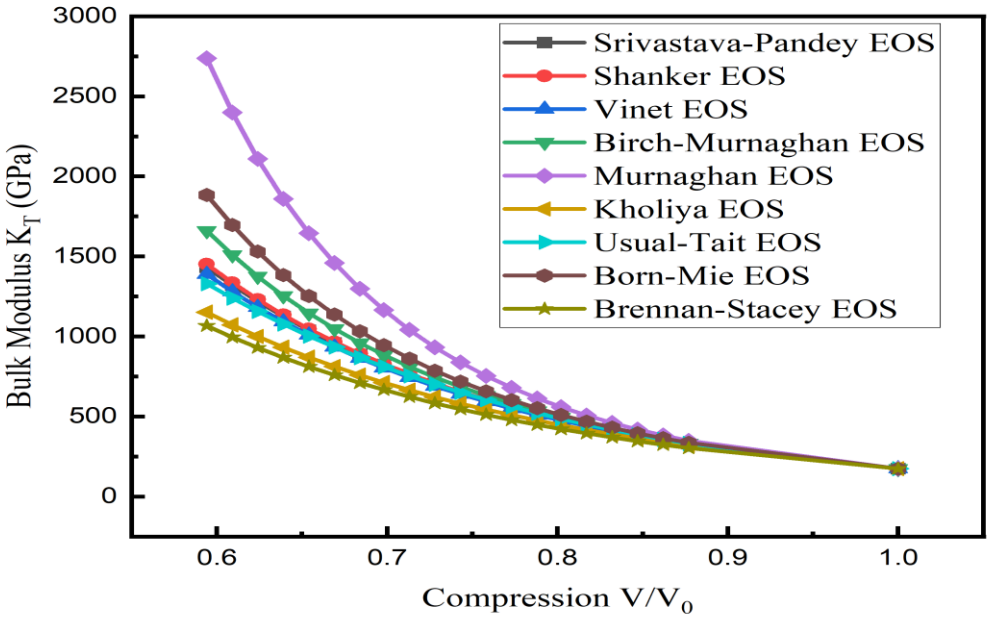

Fig. 2. Variation of bulk modulus with different compression for ε-Fe.

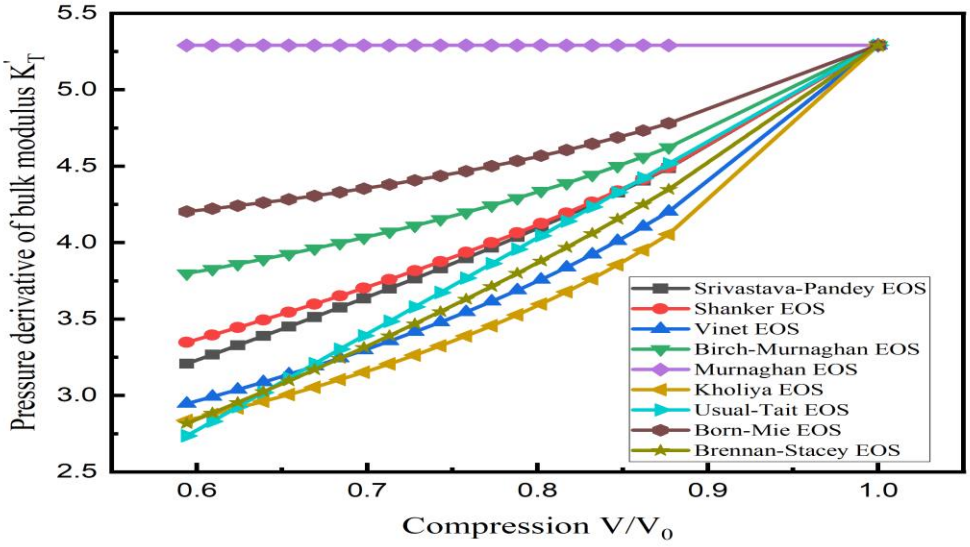

Fig. 3. Variation of pressure derivative of bulk modulus with different compression for ε-Fe.

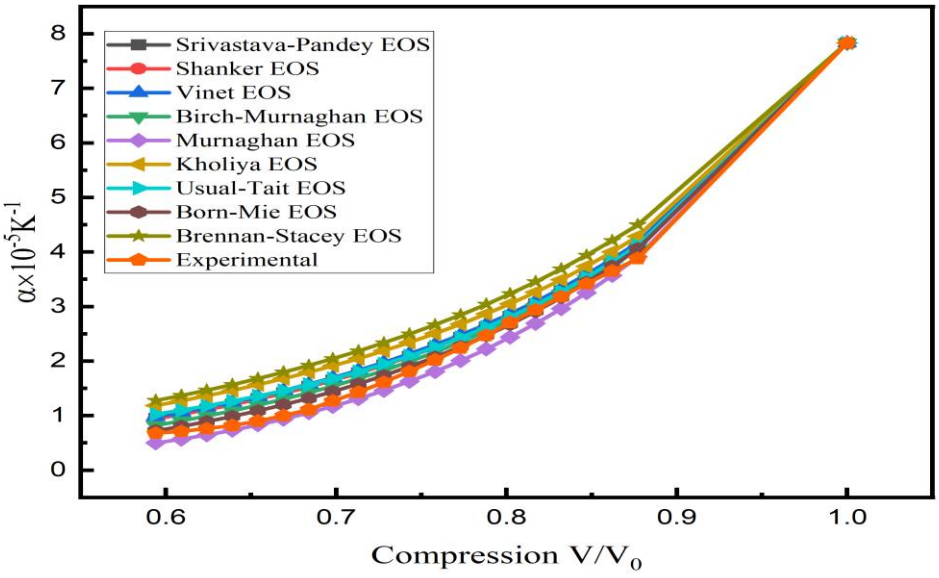

Fig. 4. Variation of volume thermal expansion coefficient with different compression for ε-Fe.

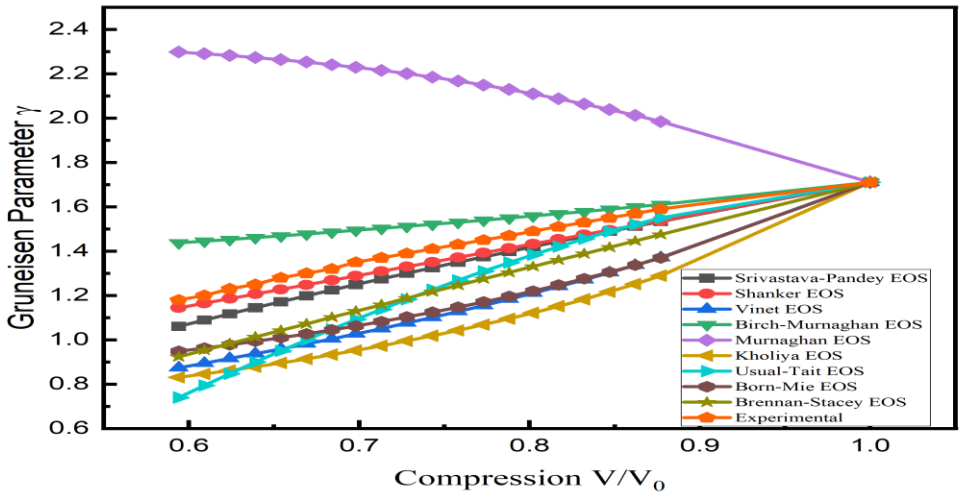

Fig. 5. Variation of Gruneisen parameter with different compression for ε-Fe.

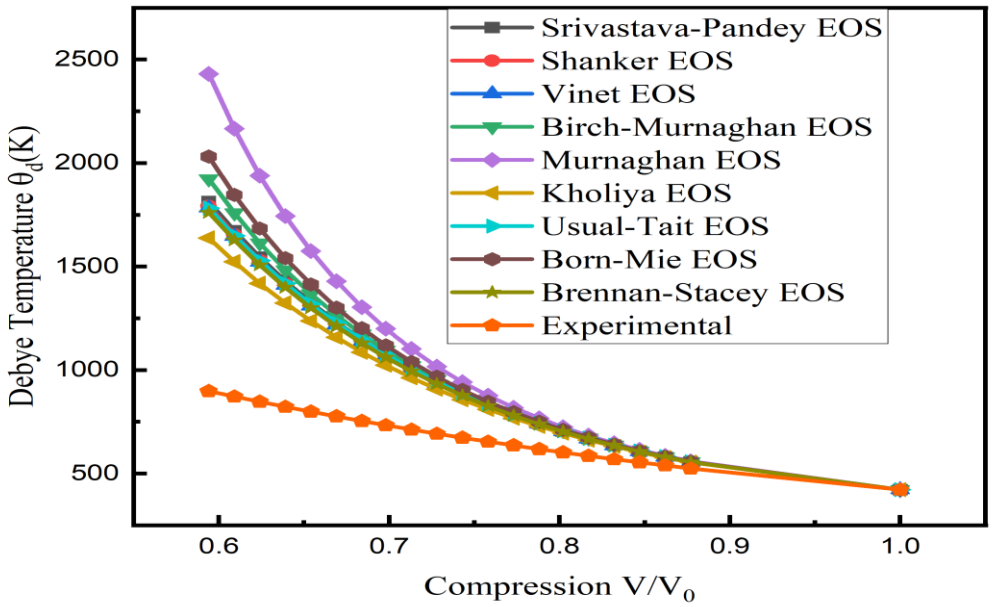

Fig. 6. Variation of Debye temperature with different compression for ε-Fe using equation (46).

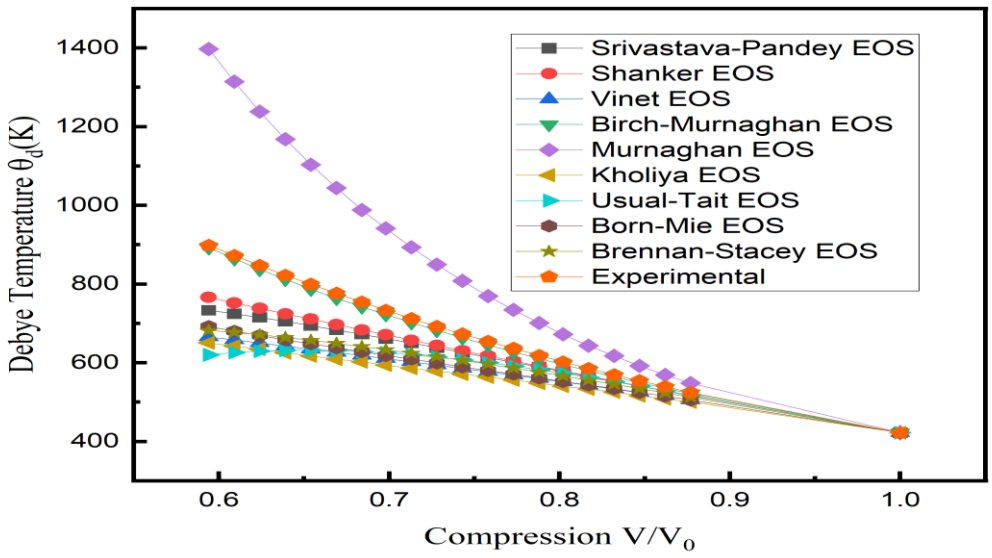

Fig. 7. Variation of Debye temperature with different compression for ε-Fe using equation (48).

2.7. Result and discussion

The following research paper provides a detailed analysis of the compression-dependent thermoelastic properties of ε-Fe. It examines various equations of state, including the Srivastava-Pandey EOS, Shanker EOS, Vinet EOS, Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Usual-Tait EOS, Born-Mie EOS, and Brennan-Stacey EOS. The formulation for the compression-dependent bulk modulus is established using equation (10) and is presented in equations (12) to (20). In addition, it determines the first-order pressure derivative of bulk modulus for all state equations using equation (11) and represents it in equations (21) to (29). The expression for the compression-dependent volume thermal expansion coefficient and Gruneisen parameter is shown in equations (32) and (33), respectively. Furthermore, equations (46) and (48) present the expression for the Debye temperature based on the Gruneisen parameter and the Debye model. The essential input parameters are shown in Table 1. The curves present the calculated values of compression-dependent pressure, bulk modulus, and first-order pressure derivative of bulk modulus with available experimental data. The calculated compression-dependent volume thermal expansion coefficient values, the Gruneisen parameter, and the Debye temperature are based on the Gruneisen parameter, and the Debye model is also compared by the curves. Finally, the paper includes figures (Fig. 1-7) that illustrate the variation of pressure, bulk modulus, first-order pressure derivative of bulk modulus, volume thermal expansion coefficient, Gruneisen parameter, and Debye temperature based on the Gruneisen and Debye models. The graph shows that as compression and pressure increase, the bulk modulus and Debye temperature also increase. Conversely, the first-order pressure derivative of bulk modulus, the volume thermal expansion coefficient, and the Gruneisen parameter all decrease. The pressure values calculated using the Birch-Murnaghan EOS, Srivastav-Pandey EOS, and Born-Mie EOS closely match the experimental values. However, deviations occur when using other equations of state for the calculations. The behavior of all equations of state is similar in the calculation of bulk modulus and the first pressure derivative of bulk modulus, except for the Birch-Murnaghan EOS, Murnaghan EOS, Kholiya EOS, Born-Mie EOS, and Brennan-Stacey EOS. The Born-Mie equation of state provides better results for calculating the volume thermal expansion coefficient, and deviations occur in the computation with other equations of state. Still, the Srivastava-Pandey EOS, Shanker EOS, and Birch-Murnaghan EOS also give good results with a slight deviation. Regarding the calculation of compression-dependent Gruneisen parameter, Srivastava-Pandey EOS and Shanker EOS are very close to the experimental values, but others deviate significantly. The calculated values of Debye temperature by the Gruneisen parameter are much deviated for all equations of states with experimental values. Still, based on the Debye model, the

calculation is much closer to the experimental result, shown in Fig. 6 and Fig. 7. The expression for the Gruneisen parameter based on the Gruneisen theory is pressure dependent. In contrast, the Debye model depends upon compression and the Gruneisen parameter. The deviation in the result obtained for the Gruneisen parameter by all equations of state is minimal, and in the case of pressure, the deviation is significant; therefore, the deviation is also large in Debye temperature by the Gruneisen parameter model. The nature of the curve for compression-dependent Debye temperature is a straight line according to the experimental calculation. Still, it is exponential if we calculate by equation (46) and significant deviation. Calculation by the Debye model shows a similar pattern to the experimental one, and in this case, Birch-Murnaghan EOS good resembles the experimental result. The Srivastava-Pandey and Shanker EOS also give better results than the other equations of states. In this study, we analyze Birch-Murnaghan EOS, Srivastava-Pandey EOS, Shanker EOS, and Born-Mie EOS as being more suitable than other equations of states. These are higher-order equations of states, suggesting we can increase the accuracy of the equation of state by increasing the order of compression in the equation of state. Birch-Murnaghan is most suitable in all cases, as the region contains higher-order compression and is balanced with attractive and repulsive potential with increasing compression. Srivastava-Pandey EOS and Shanker EOS are also best for calculating thermophysical properties. Still, at higher compression, there is a significant deviation because, in the derivation of Srivastava-Pandey EOS and Shanker EOS, only the exponential behavior of the solid is considered. Still, at higher compression, the potential structure of the solid is perturbed. Redistribution of potential suggests a need for an equation of state that can work at higher compression and successfully predict the thermophysical property of solids in perturbed potential conditions.

2.8. Conclusion

In this study, we calculated the thermoelastic properties of ε-Fe up to 359.5 GPa and compared them with available experimental data. Our analysis concludes that a higher-order equation of state effectively predicts the thermoelastic properties of solids. This suggests the necessity of developing a new equation of state that balances attractive and repulsive energy terms under high compression. While equations derived with low-order compression and only attractive potentials adequately explain solid behavior at low compression, incorporating attractive and repulsive terms is crucial at high compression.

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

Competing interests:

The individuals who authored this paper state that they do not possess any known financial interests or personal relationships that could have potentially influenced the work presented in this report.

Author's Contribution:

All authors participated in creating the research outline. Abhay P. Srivastava completed all calculations and the initial manuscript draft. Professor B. K. Pandey provided resources and guidance throughout the project.

Funding:

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

Availability of data and Materials:

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

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