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# Formulation of a Compression-Dependent Volume Thermal Expansion Coefficient Utilising the Equation of State

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## Abstract:

A comprehensive theoretical formulation has been developed to investigate the impact of compression on solid materials' volume thermal expansion coefficient. The volume thermal coefficient depends solely on three key factors: the pressure that varies with compression, the material's bulk modulus at zero pressure, and the first derivative of the bulk modulus concerning pressure at zero pressure. To validate this theoretical approach, computed values obtained from the formulation are meticulously compared with available experimental data. The results reveal a strong correlation between the calculated values and experimental observations, thereby demonstrating the robustness and accuracy of the proposed formulation in describing the behaviour of solids under compression.

**Keywords:** Equation of state, Volume thermal expansion coefficient, Compression, hcp-iron

## Introduction:

It's thought that hexagonal close-packed (hcp) iron is the primary phase in the Earth's inner core, where we find pressures above 330 GPa and temperatures climbing to thousands of kelvins. Accurate knowledge of the Earth's thermodynamic qualities under these extreme conditions becomes essential for understanding its interior, its structure, dynamics, and how it changes. Thermal expansivity, in both volume and pressure forms, is especially critical; it effectively governs the material's response to temperature changes when volume or pressure is constrained [1-4].

The volume thermal expansivity (α) tells you the fractional volume change as temperature shifts at constant pressure. On the other hand, pressure thermal expansivity (β) defines how pressure changes with temperature at constant volume. These properties are essential when interpreting seismic data, modelling geodynamic processes, and pinpointing planetary cores' thermal state. However, and this is important, both α and β are known to respond to pressure, particularly in transition metals like iron, where compression affects bonding and electronic structure [5-9].

Although many experiments and calculations have been conducted, our comprehensive understanding of expansivity evolving with compression is still incomplete [10]. Prior research often examines expansivity at given pressures or temperatures without capturing how it depends on finite strain. We use an equation of state, or EOS, approach to tackle this gap. This lets us methodically derive hcp-iron's pressure and volume thermal expansivities under compression [11-12].

Think of it this way: we can extract vital thermodynamic parameters by fitting energy-volume data from experiments to EOS models, like the Srivastava-Pandey EOS [13], Brennan-Stacey EOS [14] and Usual-Tait EOS [15]. Then, we can analyse how these parameters evolve as pressure rises. This allows us to rigorously quantify exactly how compression affects the volume thermal expansion coefficient, which, in turn, provides new insights into how iron behaves at high pressures. Ultimately, our results help improve planetary interior modelling and support a broader understanding of matter under extreme conditions.

**Theoretical Analysis:**

If the solid is crystalline and has uniform deformation in all directions, then the volume thermal expansion coefficient and volume are related as [16]:

$$\alpha \propto V^{\lambda} \tag{1}$$

At zero pressure, equation (1) can be written as:

$$\alpha_0 \propto V_0^{\lambda} \tag{2}$$

From equations (1) and (2),

$$\frac{\alpha}{\alpha_0} = \left(\frac{V}{V_0}\right)^{\lambda} \tag{3}$$

This linear form, which does not include the exponent of λ, remains approximately valid primarily under conditions of minor strains or within the context of specific empirical fits observed in anisotropic or layered systems. In such cases, the volume change tends to align linearly with the lattice change in a given direction. However, it is essential to note that this linear approximation does not hold from first principles under more general conditions. Equation (3) can be modified as:

$$\alpha = \alpha_0 \left(\frac{V}{V_0}\right)^{\lambda} \tag{4}$$

For solid material and non-linear expansion $\lambda = K_0'$ Then, equation (4) can be written as:

$$\alpha = \alpha_0 \left(\frac{V}{V_0}\right)^{K_0'} \tag{5}$$

Now, we consider the three-isothermal equations of state, such as the Srivastav-Pandey equation of state [17-18], which is derived based on the Gruneisen approximation, the Brennan-Stacey equation of state

[18], which is derived based on the semi-empirical method, and the Usual-Tait equation of state [19], which is derived based on the empirical theory, represented by equations (5), (6), and (7).

$$P = K_0\left(\frac{V}{V_0}\right)^{-4/3} \times \left[\frac{\left\{a^3(1+q+q^2+q^3)+a^2(-3q^2-2q-1)+a(6q+2)-6\right\}e^{aq}-(a^3-a^2+2a-6)}{a^4}\right] \tag{6}$$

Where P is compression-dependent pressure, $K_0$ Is the bulk modulus at zero pressure? $K_0'$ is the first-order pressure derivative of the bulk modulus at zero pressure, $V/V_0$ is volume compression, $a = \frac{3K_0'-8}{3}$ and $q = 1 - \frac{V}{V_0}$.

$$P = \frac{3K_0\left(\frac{V}{V_0}\right)^{-\frac{4}{3}}}{\left(3K_0'-5\right)}\left[\left\{\exp\left(\frac{3K_0'-5}{3}\right)\left(1-\frac{V}{V_0}\right)\right\}-1\right] \tag{7}$$

and

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

The inverted type equation of state corresponding to the Srivastava-Pandey equation of state can be expressed as:

$$\frac{V}{V_0} = 1 - \left[\frac{-1+\sqrt{1+\frac{4\eta P}{K_0}}}{2\eta}\right] \quad \text{where } \eta = \left\{\frac{\left(K_0'-2\right)(6K_0'-5)}{6}\right\} \tag{9}$$

The expression corresponding to the Srivastava-Pandey equation of state, expressed as:

$$\alpha = \alpha_0\left[1-\left\{\frac{-1+\sqrt{1+\frac{4\eta P}{K_0}}}{2\eta}\right\}\right]^{K_0'} \quad \text{where } \eta = \left\{\frac{\left(K_0'-2\right)(6K_0'-5)}{6}\right\} \tag{10}$$

The expression for the volume thermal expansion coefficient corresponding to the Brennan-Stacey and the Usual-Tait equation of state, expressed as:

$$\alpha = \alpha_0 \left[ 1 - \left\{ \frac{-1 + \left( 1 + \frac{4\beta P}{K_0} \right)}{2\beta} \right\} \right]^{K_0'} \text{ where } \beta = K_0' - \frac{7}{3}. \tag{11}$$

$$\alpha = \alpha_0 \left| 1 - \frac{1}{K_0' + 1} \ln \left[ \frac{\left\{ P\left( K_0' + 1 \right) + K_0 \right\}}{K_0} \right] \right|^{K_0'} \tag{12}$$

Equations (6), (7), and (8) allow us to calculate the compression-dependent pressure, and equations (10), (11), and (12) allow us to calculate the solids' compression-dependent volume thermal expansion coefficient.

## Result and Discussion:

In this study, we estimate the compression-dependent pressure by using equations (6), (7), and (8) and draw the curve, which is shown in Fig. 1, and for better clarity, compare the computed result with experimental data [21, 22]. The estimation of compression-dependent volume thermal expansion coefficient is done by using equations (10), (11), and (12), and drawing the curve shown in Figure 2, and for clarity, comparing the computed values with experimental data [21]. The input values used in the calculation are the bulk modulus at zero pressure. $K_0$=174 GPa and its pressure derivative $K_0'$=5.29 [20].

Fig. 1 shows that pressure increases with the increase in compression. The computed pressure values by the Srivastava-Pandey EOS are very close to the experimental values. Still, the results obtained by Brennan-Stacey and Usual-Tait deviate significantly from the experimental values. Srivastava-Pandey, Brennan-Stacey, and Usual-Tait are exponential equations of state, but the Srivastava-Pandey equation of state contains a higher order of compression, which increases its accuracy.

Fig. 2 shows that the volume thermal expansion coefficient decreases with increased compression. The equation that gives the pressure values with better accuracy also gives high-accuracy values of the volume thermal expansion coefficient. The values of the volume thermal expansion coefficient computed by the Srivastava-Pandey equation of state are more accurate than others and lie above the experimental curve. Still, values calculated by the Usual-Tait equation give values with slightly less accuracy and lie below the experimental curve. The deviation is more in the calculated values by the Brennan-Stacey equation of state. The values computed by the Srivastava-Pandey equation of state are slightly higher than experimental values at high pressure because its formulation of volume thermal expansion coefficient depends upon the second order of pressure derivative of bulk modulus. In contrast, other formulations rely only on the first order of the pressure derivative of bulk modulus. From the above discussion, it is clear that the Srivastava-Pandey equation of state is suitable for predicting thermophysical properties of solids.

## Conclusion:

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In this study, we formulate a formula for the compression-dependent volume thermal expansion coefficient using three different equations of state: the Srivastava-Pandey equation of state, the Brennan-Stacey equation of state, and the Usual-Tait equation of state. After thoroughly analysing, it is clear that the equation of state, which contains a higher order of compression, is suitable for predicting the thermophysical properties of solids.

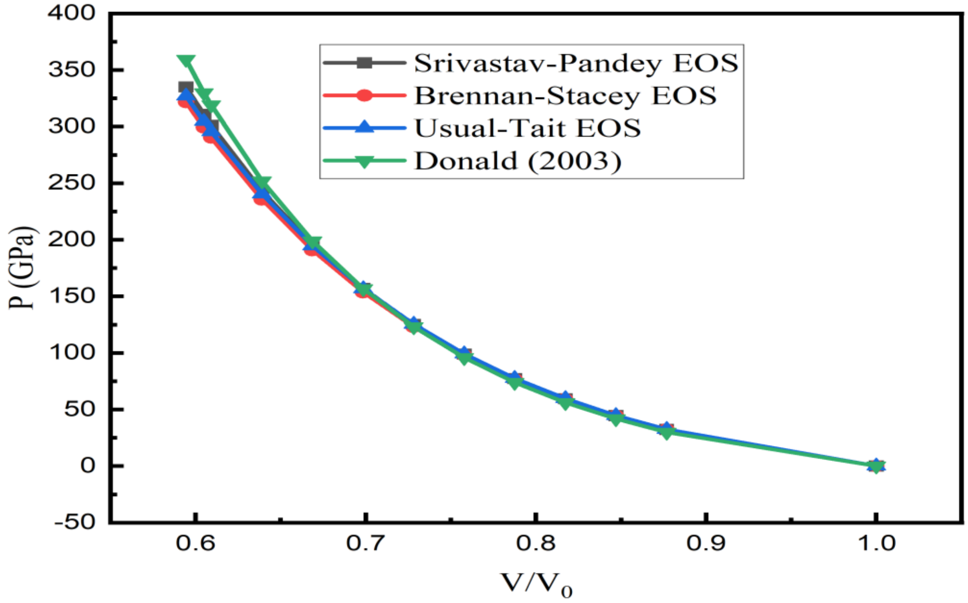

**Fig. 1.** Compression-dependent pressure of hcp-iron

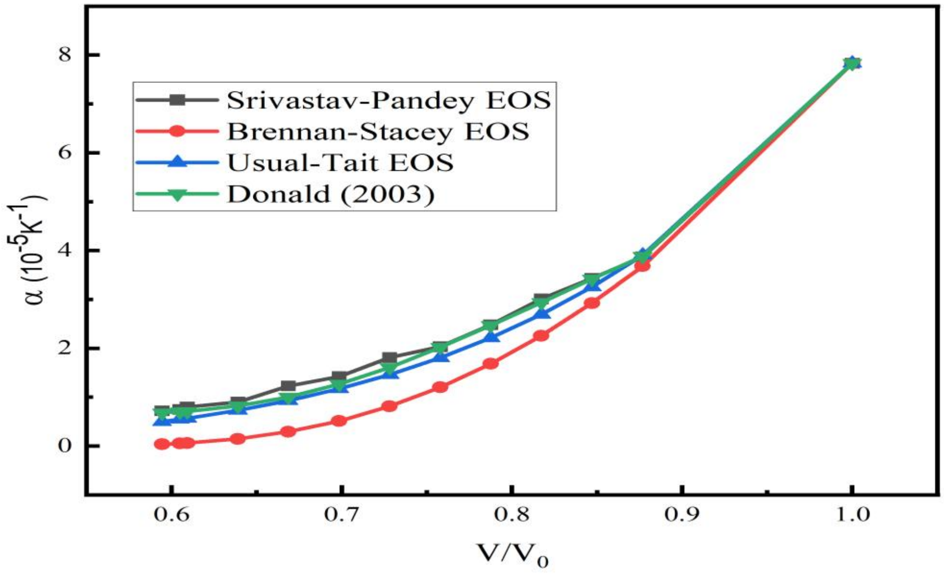

**Fig. 2.** Compression-dependent volume thermal expansion coefficient of hcp-iron

## Ethical Approval:

The authors confirm that the manuscript is original and unpublished.

## Competing interests:

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

## Author's Contribution:

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

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