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Formulation for the melting temperature of alkali halides using the equation of state under varying pressure

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Abstract

This work primarily focuses on predicting the equation of state required to compute the pressure-dependent melting curves of alkali halides. In this work, we propose developing models to describe the melting curve using the Murnaghan, Singh, Kao, Shanker, and Usual-Tait equations of state. Our model explicitly describes the relationships among pressure, bulk modulus, the pressure derivative of bulk modulus, and volume compression. The methodical application of theoretical models to the alkali halides yielded rigorous results that were painstakingly compared with Lindemann's model to determine the melting temperature. It is shown unambiguously in our work that a significant increase in melting temperature follows from a large increase in bulk modulus and a slight decrease in the rate of the first-order pressure derivative of bulk modulus. This work provides incredible insights into the fundamental mechanisms underlying the influence of pressure on melting temperature. We have verified that our model is unambiguously reliable in extrapolating melting temperature to high pressure.

Keywords: Equation of State, Melting Temperature of Halide, Compression, Bulk Modulus, Pressure derivative of bulk modulus.

1. Introduction

Solids under severe pressure and temperature conditions have long been at the center of concepts in condensed matter and materials science. High-pressure melting, for instance, is very important in shock wave physics, geophysics, astrophysics and nuclear physics, which involves materials that experience intense thermodynamic environments. The responses of solids to compression and the eventual liquid phase can contribute to an understanding regarding the internal structure of planetary bodies and how impact events unfold, and materials behavior and stability in extreme technological scenarios [1-3].

For over 20 years the physical and chemical properties of solids in high pressures have attracted much theoretical and experimental attention. A range of thermodynamic models and schemes have been proposed in order to characterize such systems more clearly. More sophisticated methods, such as complex differential expressions and thermodynamic methods have allowed a more comprehensive understanding of the pressure–volume–temperature relationships and phase-stability characteristics concerning compression [4-6].

At the core of these explorations is the equation of state (EOS), a fundamental relationship that integrates pressure, volume (or density), and temperature. The EOS offers quantifiable tools to describe the compressive capacity of a material under applied pressure, in addition to how its thermodynamic properties evolve. An EOS provides key

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parameters including the bulk modulus, its first pressure derivative, and the volume compression. Such quantities are fundamental for describing mechanical stability and elastic response. More important, equations of state enable scientists to investigate pressure ranges that can be experimentally unfeasible or even impossible to measure [7-9].

Experimental methods like the diamond-anvil cell (DAC), forced high pressure X-ray diffraction and shock wave compression have given essential high-pressure information, but are still hampered by technical and engineering restrictions. Thus, theoretical approaches including molecular dynamics simulations, ab initio simulations and semi-empirical thermodynamic models are essential complementary instruments. The Lindemann–Gilvarry criterion-based models further link the vibrational properties to the melting behavior in terms of the dynamical behavior and provide a simplified yet physically meaningful description of melting under compression [10-12].

Theory models of high-pressure melting curves are expected to be derived, satisfying a rigid thermodynamic condition (the Gibbs free energies of the solid and liquid phase at the melting point equal). It is still difficult to solve this problem because atomic arrangements and interatomic interactions are complex in either. The liquid phase has no long-range order, and a pressure dependence of vibrations and anharmonic effects makes it even more complicated. Among the more simplified approaches, Lindemann's law provides a good approximation for the pressure dependence of melting temperature from the vibrational amplitudes and Grüneisen parameter [13-15].

Such formulations must be based upon the Grüneisen parameter at reference conditions and its change with compression. The goal of this work is to derive and evaluate an accurate isothermal equation of state to determine melting temperatures under compression [16-18]. Experimentally determined zero-pressure bulk modulus (K_0) and its first pressure derivative (K_0') are used as input factors. With the quantities above, the melting temperature could be observed across a range of pressures, especially for alkali halides. Different kinds of thermodynamic formulas and state equations are cross-referenced with the existing theoretical data in order to develop a consistent set of theories for pressure-related melting processes.

2. Methodology and Analysis

The melting temperature of solids at different ranges of pressure can be obtained by the equation of state (EOS), such as

2.1. Murnaghan Equation of State: Murnaghan proposed the equation of state based on the linear dependence of the isothermal bulk modulus on pressure for solids, which may be written as [19]

$$P = \frac{K}{K_0^{'}}\left[\left(\xi\right)^{-K_0^{'}} - 1\right] \tag{1}$$

Where P is compression-dependent pressure, K_0 is the bulk modulus at zero pressure, K_0' is the first-order derivative of the bulk modulus at zero pressure and $\xi = \frac{V}{V_0}$ is volume compression.

The bulk modulus is defined as

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

Differentiating equation (1) with respect to volume, the isothermal bulk modulus K can be expressed as:

$$K = K_0\left(\xi\right)^{-K_0^{'}} \tag{3}$$

The first-order derivative of the bulk modulus for pressure is given by

$$K^{'} = \left(\frac{dK}{dP} \right) \tag{4}$$

Using equations (3) and (4), the first-order pressure derivative of the bulk modulus is expressed as:

$$K' = \frac{K_0 K_0^{'}}{K} \left(\xi \right)^{-K_0^{'}} \tag{5}$$

The inverted form of the isothermal equation (1) can be expressed in terms of $\frac{V}{V_0}$ as:

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

Equation (6) calculates volume compression, which is proportional to the pressure.

The thermal pressure P_{th} is expressed as [20-21]

$$P_{th} = \int_{T_0}^{T} \alpha K dT \tag{7}$$

Where α is thermal expansivity, T_0 is room temperature, and T is elevated temperature.

Integrating equation (7) then thermal pressure can be expressed as:

$$P_{th} = \alpha K (T - T_0) \tag{8}$$

Thermal pressure at zero pressure is expressed as

$$P_{th} = \alpha_0 K_0 (T - T_0) \tag{9}$$

From equations (6) and (7), the expression for the melting temperature of solids can be obtained as:

$$T_{mo} - T_0 = \frac{K K_0^{'}}{\alpha_0 K_0 K^{'}} \tag{10}$$

To obtain the melting temperature of a solid at pressure P, terms including K_0' and K_0 in equation (10) must be replaced by K' and K then the equation (10) becomes:

$$T_m(P) = T_0 + (T_{m0} - T_0) \frac{K K_0^{'}}{K_0 K^{'}} \left(\xi \right) \tag{11}$$

2.2. Singh and Kao Equation of state: The Singh and Kao equation of state is expressed as [22]

$$P = K_0 \left(1 - \xi \right) + \left\{ \frac{K_0 (K_0^{'} + 1)}{2} \right\} \left(1 - \xi \right)^2 \tag{12}$$

The bulk modulus and first-order derivative of the bulk modulus corresponding to the Singh and Kao equation of state are expressed as

$$K = \xi K_0 \left[1+\left(K_0^{'}+1\right)-\left(K_0^{'}+1\right)\xi\right] \tag{13}$$

$$K^{'} = \frac{K_0}{K}\xi\left[-1-(K_0^{'}+1)+2(K_0^{'}+1)\xi\right] \tag{14}$$

Similarly, the expression for volume compression and melting temperature corresponds to Singh and Kao's equation of state, which can be expressed as

$$\xi = 1-\left[\frac{-1+\sqrt{1+\frac{2(K_0^{'}+1)P}{K_0}}}{K_0^{'}+1}\right] \tag{15}$$

$$T_m(P) = T_0 + (T_{m0}-T_0)\frac{\left(K_0^{'}+1\right)}{\left(K^{'}+1\right)}\xi \tag{16}$$

2.3. Shanker equation of state: Considering the Born lattice theory and deriving the volume derivative of the short-range force constant, Shanker obtained an equation of state known as Shanker EOS [23].

$$P = \frac{3K_0(\xi)}{\left(3K_0^{'}-8\right)}^{-\frac{4}{3}}\left[\left\{\left(1-\frac{1}{t}+\frac{2}{t^2}\right)\left(\exp ty-1\right)\right\}+\left\{y\left(1+y-\frac{2}{t}\right)\exp ty\right\}\right] \tag{17}$$

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

The expression for bulk modulus, the first-order derivative of bulk modulus, volume compression, and melting temperature corresponding to the Shanker equation of state is expressed as:

$$K = \frac{4}{3}P + K_0(\xi)^{-\frac{4}{3}}\exp\left\{\left(K_0^{'}-\frac{8}{3}\right)(1-\xi)\right\} \tag{18}$$

$$K^{'} = \frac{16}{9}\frac{P}{K}+\left(1-\frac{4}{3}\frac{P}{K}\right)\left[\left\{\left(K_0^{'}-\frac{8}{3}\right)(\xi)\right\}+\frac{8}{3}\right] \tag{19}$$

$$\xi = 1+\frac{1-\sqrt{1+\frac{2(K_0^{'}+1)P}{K_0}}}{K_0^{'}+1} \tag{20}$$

$$T_m(P) = T_0 + (T_{m0} - T_0)\frac{K\left(K_0^{'}+1\right)}{K_0(K^{'}+1)}\xi \tag{21}$$

2.4. Usual-Tait equation of state: Usual-Tait proposed a new EOS, known as Usual-Tait EOS, with a slight modification in Murnaghan EOS as [24]:

$$P = \frac{K_0}{\left(K_0^{'}+1\right)}\left[\exp\left\{\left(K_0^{'}+1\right)(1-\xi)\right\}-1\right] \tag{22}$$

The expression for bulk modulus, the first-order derivative of bulk modulus, volume compression, and melting temperature corresponding to Shanker equation of state is expressed as:

$$K = K_0(\xi)\exp\left\{\left(K_0^{'}+1\right)(1-\xi)\right\} \tag{23}$$

$$K^{'} = \frac{\left(K_0^{'}+1\right)(2\xi-1)-1}{\left(K_0^{'}+1\right)(1-\xi)+1} \tag{24}$$

$$\xi = 1-\frac{1}{K_0^{'}+1}\left[\frac{\ln\left\{P\left(K_0^{'}+1\right)+K_0\right\}}{K_0}\right] \tag{25}$$

$$T_m(P) = T_0 + (T_{m0} - T_0)\frac{K\left(K_0^{'}+1\right)}{K_0(K^{'}+1)}\xi \tag{26}$$

We may determine the bulk modulus of alkali halides using equations (3), (13), (18), and (23). These equations are crucial tools for understanding the material's response to stress. In addition to that, equations (5), (14), (19), and (24) will also be used to find the pressure derivative of the bulk modulus to examine the bulk modulus response to pressure. Besides that, from equations (6), (15), (20), and (25) we can apply the material's compression according to a particular pressure, P, and finally, from equations (11), (16), (21), and (26) we can determine the melting temperature of alkali halides at pressure P. We can systematically investigate the physical properties of these compounds as a function of pressure.

Table 1 Values of input data for alkali halides [25,26]

Sample	K_0 (GPA)	K_0'	TMO(K)
LIF	66.51	5.31	1115
LiCl	29.68	5.63	887
LIBR	23.52	5.68	820
LII	16.8	4.3	723
NAF	46.5	5.28	1261
NaCl	24	5.35	1074
NaBr	19.9	5.46	1028
NAI	15.1	5.59	924
KF	30.22	5.36	1119
KCl	17.35	5.48	1049
KBr	14.64	5.48	1003

KI	11.51	5.48	959
RBF	26.68	5.69	1048
RBCL	15.58	5.62	988
RBBR	13.24	5.59	955
RBI	10.49	5.6	915

3. Result and Discussion

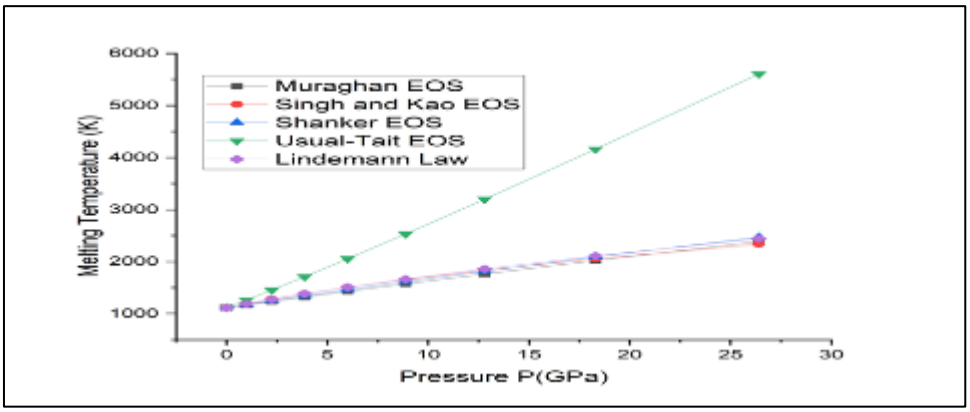

Figure 1 Pressure-dependent melting temperature of LIF

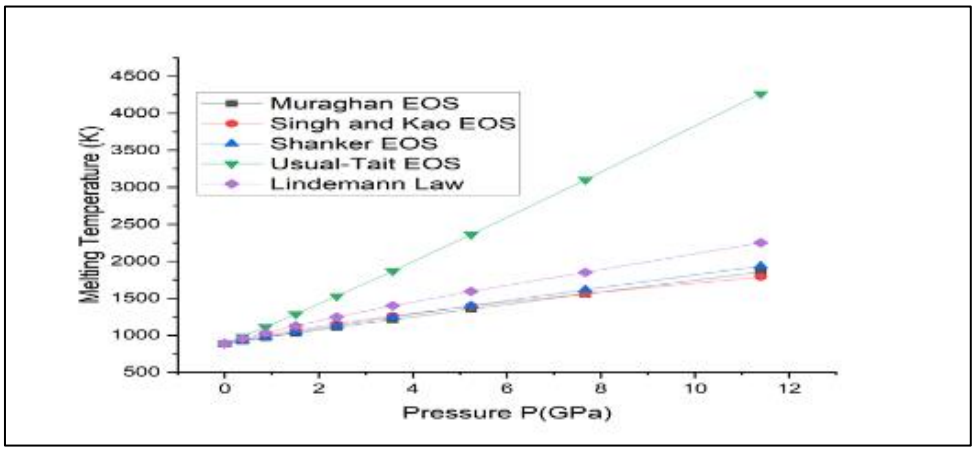

Figure 2 Pressure-dependent melting temperature of LiCl

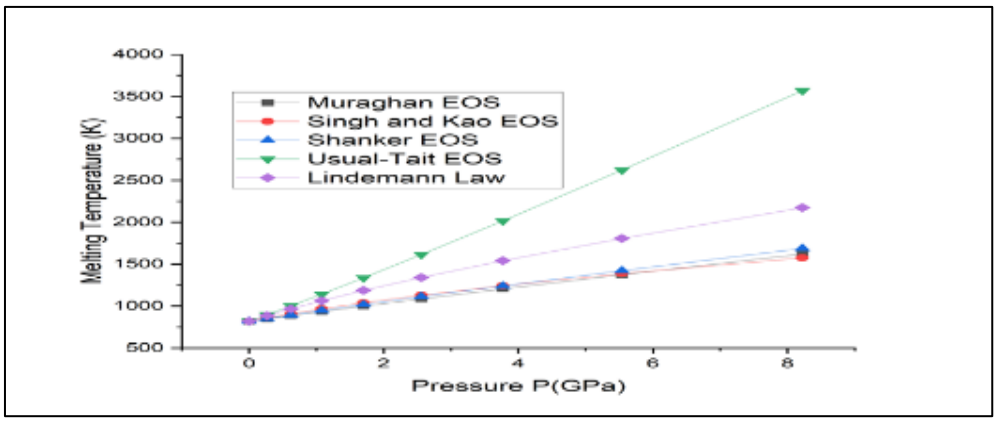

Figure 3 Pressure-dependent melting temperature of LIBR

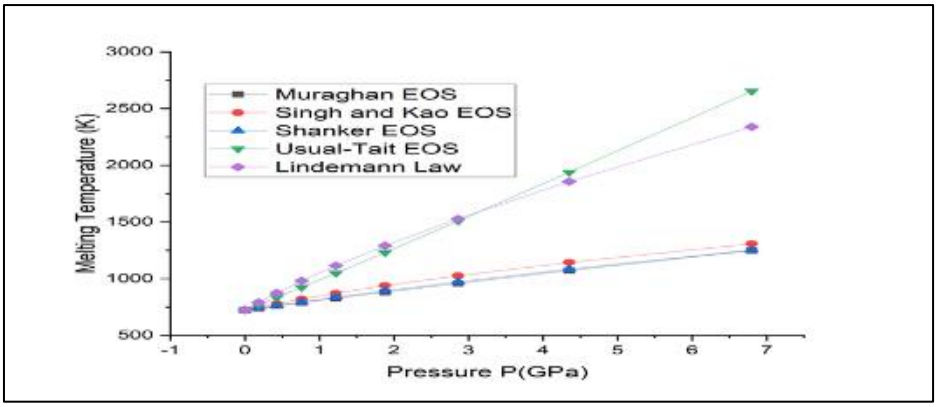

Figure 4 Pressure-dependent melting temperature of LII

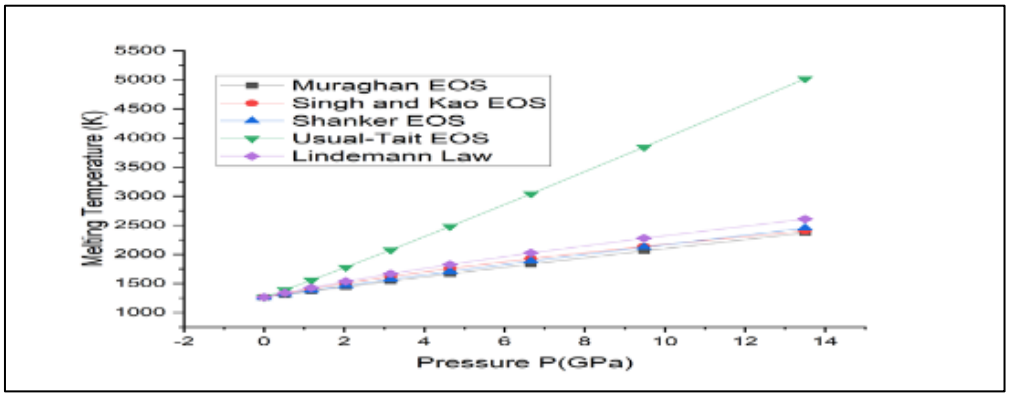

Figure 5 Pressure-dependent melting temperature of NAF

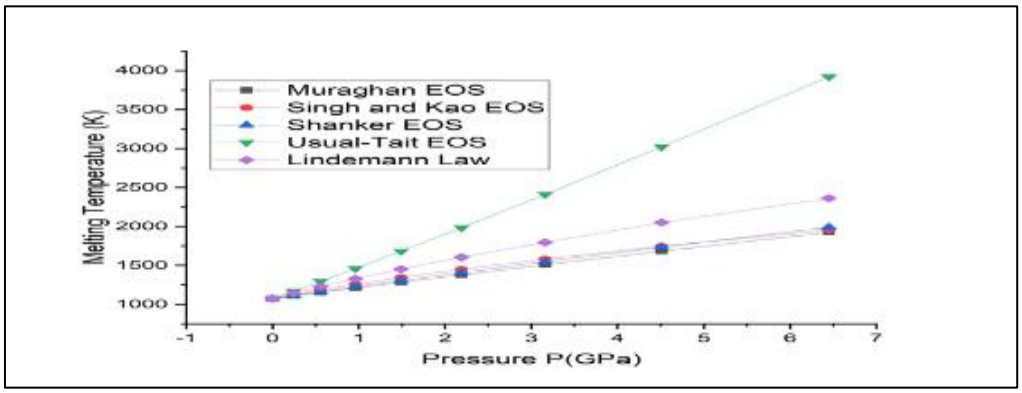

Figure 6 Pressure-dependent melting temperature of NaCl

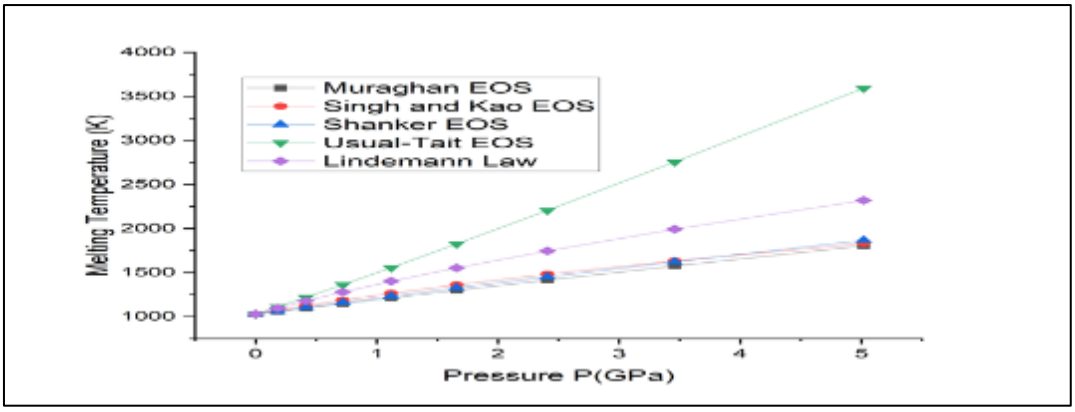

Figure 7 Pressure-dependent melting temperature of NaBr

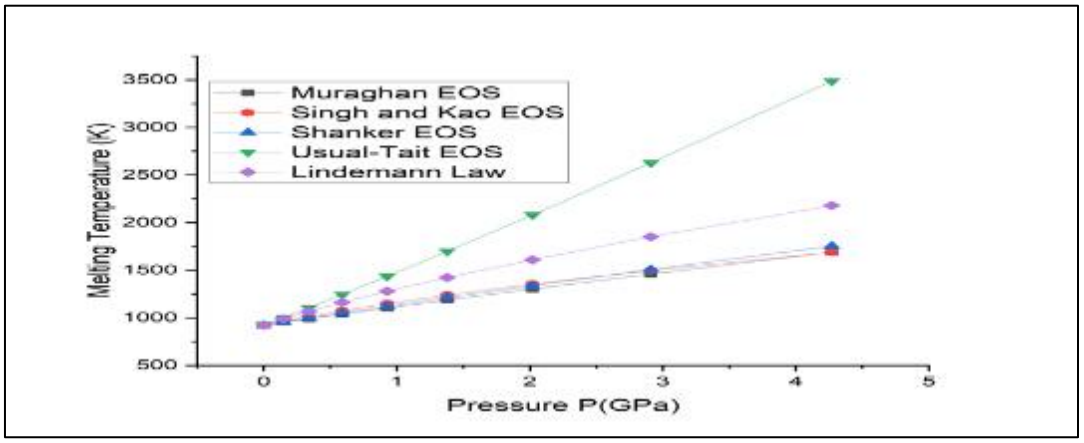

Figure 8 Pressure-dependent melting temperature of NAI

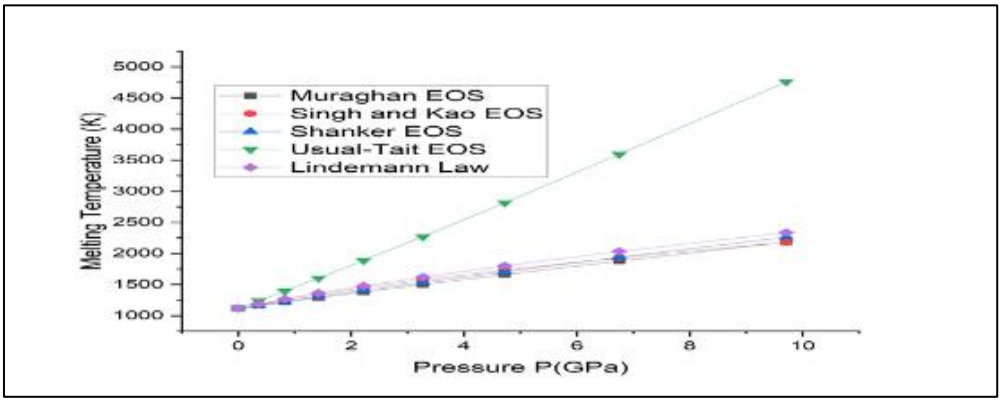

Figure 9 Pressure-dependent melting temperature of KF

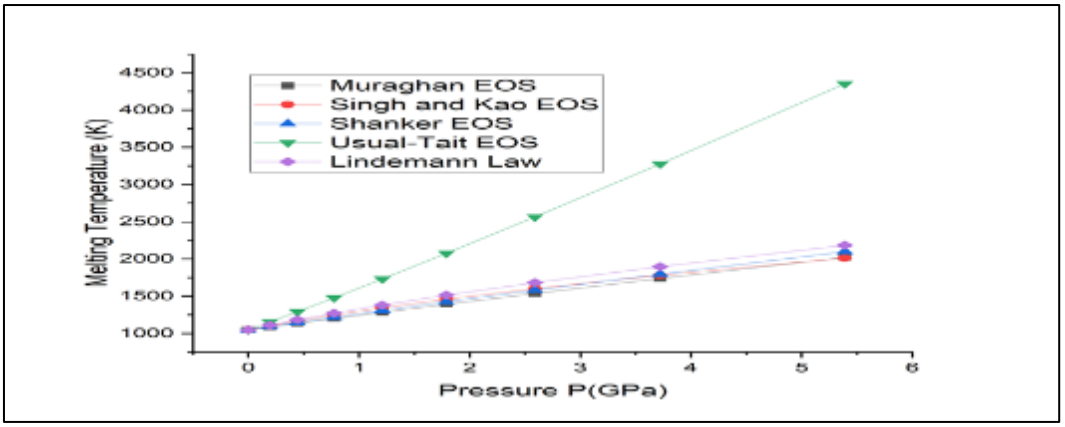

Figure 10 Pressure-dependent melting temperature of KCl

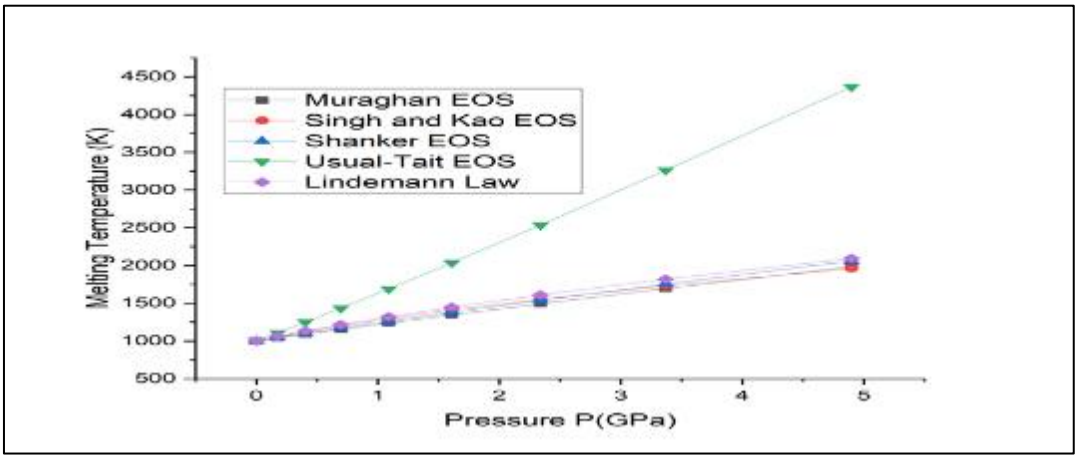

Figure 11 Pressure-dependent melting temperature of KBr

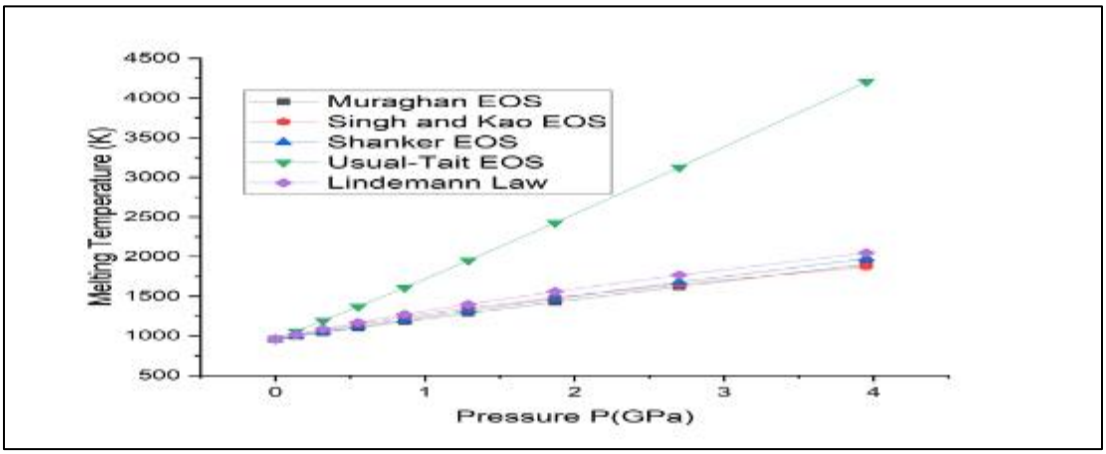

Figure 12 Pressure-dependent melting temperature of KI

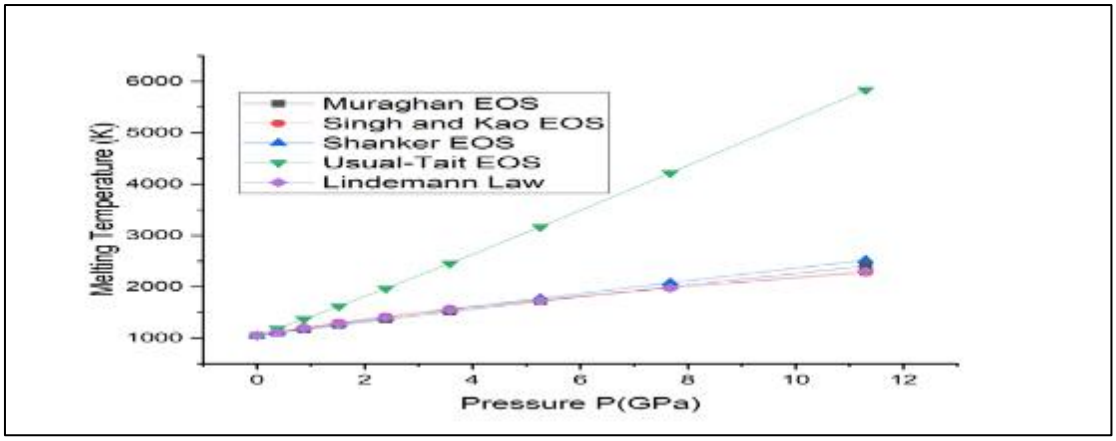

Figure 13 Pressure-dependent melting temperature of RBF

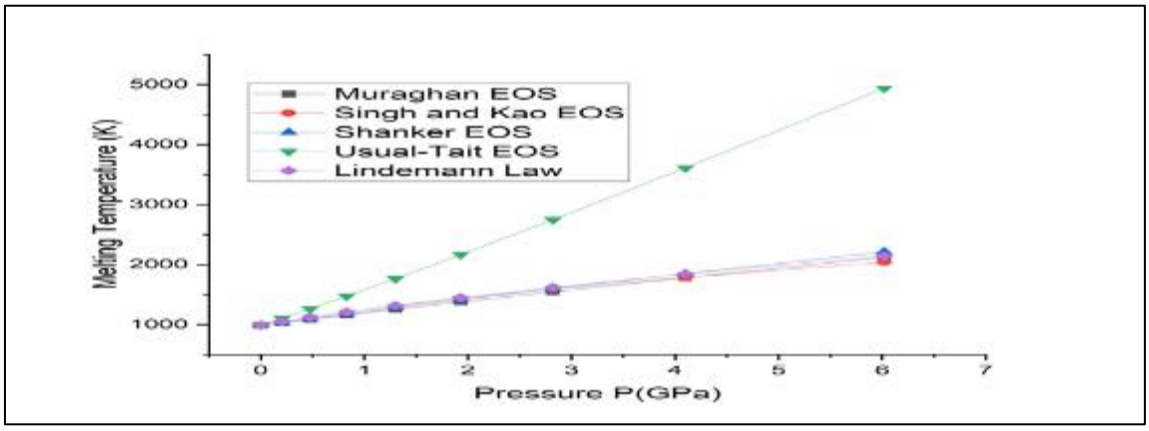

Figure 14 Pressure-dependent melting temperature of RBCL

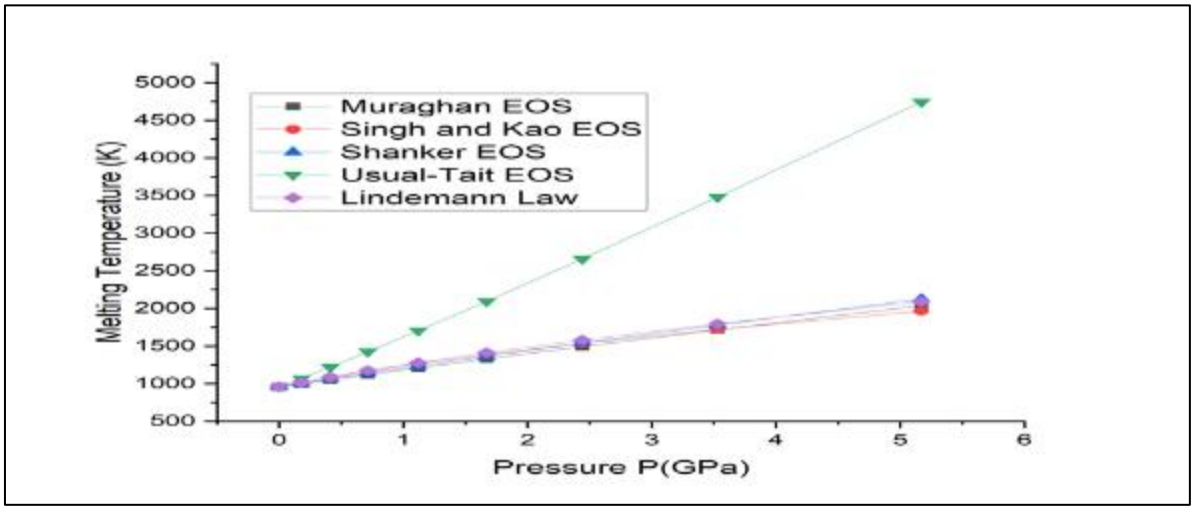

Figure 15 Pressure-dependent melting temperature of RBBR

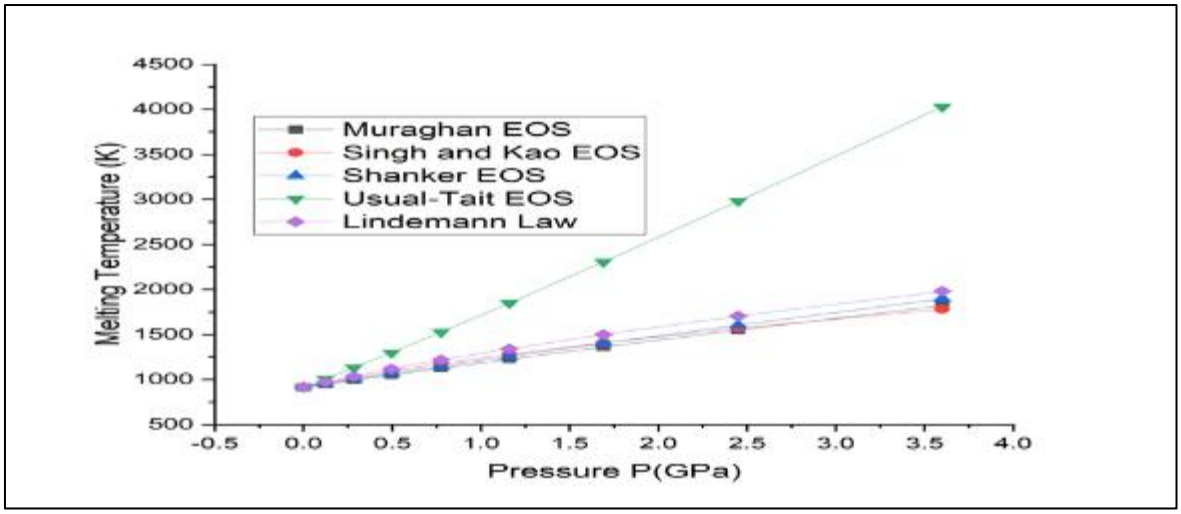

Figure 16 Pressure-dependent melting temperature of RBI

Together, they yield a thermodynamic characterization of the pressure-dependent melting response in alkali halides (LIX, NAX, KX, RBX; X = F, Cl, Br, I). Melting temperature increases monotonically with pressure in all compounds, confirming a positive melting slope [27-32].

This is consistent with the Clausius–Clapeyron relation, which states that the slope of the melting curve depends on the entropy and volume changes during the solid–liquid transition. Since alkali halides typically exhibit a positive volume change upon melting, under pressure compression leads to a stable solid-phase relative to the liquid phase, and therefore to an increasing melting temperature. A closer analysis shows systematic periodic trends. In the case of a fixed alkali metal, the temperature at which it melts decreases from fluoride to iodide. This is due to the increment of anion size ($F^- \rightarrow I^-$), which lowers the Coulombic affinity, decreases lattice energy, decreases the bulk modulus, and modulates vibrational frequencies. As a result, across the halogen series, Debye's temperature drops, and more stability in melting is lost.

Likewise, for a fixed halogen, the melting temperature decreases from lithium to rubidium because the cation radius increases ($Li^+ \rightarrow Rb^+$). Higher-weight cations lead to relatively weaker electrostatics and reduced elastic stiffness, making the lattice more compressible and less thermally stabilizing. These structural and elastic properties, therefore, are responsible for the reason(s) behind LiF having the highest melting temperature and lower RbI compared with the material evaluated. Comparing the models' performances can also yield valuable thermodynamic information. The Murnaghan, Singh–Kao, and Shanker equations of state reveal nearly linear melting curves and are well matched across the pressure range, suggesting that their compressibility descriptions are internally coherent and reasonably effective at moderate pressures.

The Lindemann law, which associates melting temperature with vibrational amplitudes and the Grüneisen parameter, indicates slightly higher melting temperatures. This indicates how it reacts to lattice vibrational stiffening in the presence of compression. On the other hand, the Usual-Tait EOS generates strongly nonlinear behavior and high melting temperatures at high pressures. This means that the Usual-Tait formulation enhances the effect of compression on elastic parameters and overestimates solid-phase stability at high pressure. In terms of application, it is necessary to explore pressure-dependent melting behavior for alkali halides in a variety of applications. Alkali halides are used as model ionic solids for modeling the melt in planetary interiors at tens of gigapascals of pressure on the planet for applications in geophysics and planetary science.

Smooth melting curves can be used to model phase stability and thermal evolution of planetary crusts and mantles. Insight into the behaviour of high-pressure melting in shock wave physics and detonation science is of paramount importance for modeling phase transitions during rapid compression. Alkali halides are widely used in optical devices, radiation detectors, high-temperature windows, and molten-salt technology in materials engineering. The behavior of these materials under pressure determines their degree of survivability in unfavorable conditions, for example, in nuclear reactors or space applications. Moreover, accurate melting estimates are essential for the design of high-temperature electrolytes and molten salt reactors, in which alkali halides can serve as flux materials or ionic conductors.

The impact of the pressure-enhanced melting stability may play a role in crystal growth systems under controlled compression, potentially benefiting optically and electronically valuable crystallinity. These results also provide valid thermodynamic trends, consistent with a periodic regime of varying crystalline crystallinity and lattice energy values; therefore, they validate or refute the limitations of the EOS-based melting formulas. The good agreement demonstrated by the Murnaghan, Singh–Kao, and Shanker EOS indicates their suitability for moderate-pressure predictions; caution should be exercised when applying the Usual-Tait EOS at the highest pressures [33].

4. Conclusion

In conclusion, this study presents a systematic thermodynamic framework for predicting the pressure-dependent melting temperature of alkali halides using various equations of state. The Murnaghan, Singh–Kao, Shanker, and Usual-Tait EOS were successfully applied to evaluate bulk modulus, its pressure derivative, volume compression, and melting behavior under compression. The results demonstrate a consistent increase in melting temperature with pressure, in agreement with the Clausius–Clapeyron relation and Lindemann's criterion. Clear periodic trends were observed across both cationic and anionic series, reflecting the role of lattice energy and elastic stiffness. Among the models, Murnaghan, Singh–Kao, and Shanker EOS provided reliable predictions at moderate pressures, while Usual-Tait showed stronger nonlinear behavior at higher pressures, highlighting important considerations for high-pressure applications.

Compliance with ethical standards

Disclosure of conflict of interest

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

Statement of ethical approval

The authors confirm that the manuscript is original and unpublished.

Author's Contribution

All the authors contribute equally to making the original draft of the paper.

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