



Research Article

Lindemann's Ratio Pressure Dependence of the Melting Temperature for Some Metals in Geothermal at High Pressure and High Temperature

Nand Kishor^{*} , Amar Kumar

Department of Physics, K. R (P. G) College Dr. Bhim Rao Ambedkar University, Agra, India

Abstract

The study of melting behavior under extreme conditions of pressure and temperature is essential for understanding the physical properties of metals within Earth's interior and industrial high-pressure applications. This research investigates the pressure dependence of the melting temperature for selected metals using Lindemann's melting law, which establishes a relationship between vibrational amplitudes of atomic lattices and melting phenomena. The Lindemann's ratio, defined as the critical amplitude of atomic vibrations relative to interatomic spacing, serves as the foundation for evaluating how pressure influences the melting process. In this study, the melting curves of metals such as iron (Fe), copper (Cu), aluminum (Al), and magnesium (Mg) are theoretically modeled under high-pressure conditions. The model incorporates modifications to Lindemann's law to account for the anharmonic effects and compressional behavior of lattice parameters at elevated pressures. Using the pressure-dependent Grüneisen parameter and the Mie Grüneisen equation of state, the variation of melting temperature with pressure is derived and analyzed. The results reveal that melting temperature increases nonlinearly with pressure for all investigated metals, consistent with experimental and geophysical observations. Iron, a major component of Earth's core, exhibits the highest melting slope due to its dense atomic packing and strong interatomic bonding. Conversely, metals with lower bulk moduli, such as magnesium, show a relatively moderate increase in melting temperature. The findings provide critical insights into the thermodynamic stability of metals under extreme conditions, supporting applications in geothermal studies, planetary modeling, and materials science. Overall, this work demonstrates that Lindemann's ratio remains a reliable theoretical framework for predicting melting behavior at high pressures, highlighting the importance of vibrational dynamics in understanding phase stability and the melting mechanisms of metals under extreme environments.

Keywords

Lindemann's Ratio, Melting Curve, High Pressure, High Temperature, geothermal, Grüneisen Parameter, Metals

1. Introduction

The study of melting behavior under varying pressures and temperatures is one of the fundamental topics in condensed

matter physics, materials science, and geophysics. The melting temperature of a substance is a crucial thermodynamic property that determines the boundary between its solid and

^{*}Correspondence: Nand Kishor (nandkishorout@gmail.com)

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liquid phases [1-4]. For metals, understanding how the melting temperature changes under extreme conditions provides valuable insights into atomic bonding, lattice dynamics, and structural stability. In particular, the pressure dependence of the melting temperature is of great importance for understanding the behavior of materials inside planetary interiors, including the Earth's mantle and core, where both high pressures and high temperatures prevail [5]. One of the most widely accepted theoretical frameworks for describing the melting behavior of solids is Lindemann's melting law, proposed by F. A. Lindemann in 1910. According to this law, a crystal melts when the amplitude of atomic vibrations reaches a critical fraction of the interatomic distance. This critical ratio, known as the Lindemann's ratio, provides a simple but powerful explanation for the onset of melting in solids [6]. Mathematically, Lindemann's law expresses the melting temperature as proportional to the square of the characteristic vibrational frequency of atoms and inversely proportional to the atomic mass. Because these quantities are directly influenced by pressure, the law can be used to predict how melting temperature changes with increasing pressure [7]. At elevated pressures, atomic vibrations are restricted due to compression of the crystal lattice. This leads to an increase in the characteristic vibrational frequency, which in turn raises the melting temperature. However, the relationship between pressure and melting temperature is not always linear [8]. At high pressures, factors such as electronic rearrangement, anharmonic effects, and phase transitions within the solid phase contribute to deviations from the simple linear trend. These effects necessitate a more refined theoretical approach that incorporates additional parameters such as the Grüneisen parameter and the Mie Grüneisen equation of state, which link thermal and elastic properties of materials [9].

In geophysical contexts, understanding melting under high-pressure conditions is critical for modeling the thermal and structural state of the Earth's interior. For instance, the melting temperature of iron, which constitutes a major part of the Earth's core, directly influences the formation and dynamics of the liquid outer core and the generation of the geomagnetic field. Similarly, the melting behavior of silicate and metallic components in the mantle and lower crust affects the mechanisms of magma generation, differentiation, and volcanic activity. Thus, accurate modeling of melting curves has far-reaching implications in explaining both natural and industrial high-temperature processes [10]. Experimentally determining melting temperatures at extreme pressures, however, is a complex and challenging task. Techniques such as the diamond anvil cell (DAC) and laser-heated experiments have been developed to simulate the conditions of thousands of degrees Celsius and gigapascal-level pressures [11]. Despite these advances, obtaining precise data remains difficult due to limitations in maintaining uniform temperature, detecting phase boundaries, and accounting for chemical interactions between the sample and surrounding materials. Therefore, theoretical

models like Lindemann's law remain invaluable tools for predicting melting behavior, particularly when experimental verification is impractical [12].

The Lindemann's criterion assumes that melting occurs when the root-mean-square amplitude of atomic vibration reaches approximately 10% of the interatomic distance. While simplistic, this assumption effectively captures the essence of melting in many metallic systems. To extend this law to high-pressure regimes, researchers have introduced modifications that account for volume compression, anharmonic effects, and the variation of vibrational frequency with pressure [13]. Using the Debye model, the Debye temperature is related to the vibrational frequency and the elastic properties of the material, both of which are affected by pressure. Consequently, by incorporating the pressure dependence of the Debye temperature, one can estimate the melting temperature as a function of pressure [14]. Several studies have validated Lindemann's law and its extensions against experimental results for a variety of metals and minerals. For example, in transition metals such as iron, nickel, and cobalt, the law accurately predicts the general trend of increasing melting temperature with pressure. In lighter metals like aluminum and magnesium, the rate of increase is smaller due to their lower atomic densities and weaker interatomic bonding [15]. Furthermore, comparison of theoretical and experimental melting curves provides insight into the limitations of the model and the need for further refinements, such as incorporating electron-phonon coupling or considering pressure-induced structural transitions [16]. In addition to its geophysical relevance, understanding pressure-induced melting behavior is essential for materials design and engineering applications. Metals subjected to high pressure and temperature are common in aerospace, nuclear, and manufacturing industries, where stability and performance depend on their ability to retain structural integrity under extreme environments. For instance, high-pressure melting data aid in selecting suitable materials for turbine blades, fusion reactors, and deep-earth drilling tools. Moreover, these studies support the development of new alloys with enhanced melting points and improved thermal stability [17].

This research aims to investigate the pressure dependence of melting temperature for selected metals including iron (Fe), copper (Cu), aluminum (Al), and magnesium (Mg) using a theoretical framework based on Lindemann's melting law [18]. By incorporating pressure-dependent parameters such as the Grüneisen coefficient and the Mie Grüneisen equation of state, the study refines the traditional Lindemann's approach to better represent high-pressure behavior. The resulting melting curves will be analyzed to understand the relationship between atomic structure, bonding strength, and melting temperature under high-pressure and high-temperature conditions [19]. In summary, Lindemann's melting law provides a foundational yet adaptable model for exploring the physics of melting under extreme conditions. Its simplicity, coupled with modern refinements, makes it a powerful theoretical tool for predicting melting behavior where direct measurements are difficult.

The present study contributes to the broader understanding of metallic melting mechanisms, offering insights applicable to both geothermal modeling and advanced material science, thereby bridging the gap between fundamental physics and practical engineering applications [20].

2. Research Methodology

The present study focuses on the theoretical investigation of the pressure dependence of the melting temperature of metals using Lindemann's melting law. The objective is to model how pressure influences melting behavior in selected metals namely iron (Fe), copper (Cu), aluminum (Al), and magnesium (Mg) under high-pressure and high-temperature (HPHT) conditions relevant to both industrial and geophysical environments. The methodology combines fundamental thermodynamic principles with empirical relations to establish a pressure-dependent melting curve for each metal [21].

2.1. Theoretical Framework

The study is based on Lindemann's melting criterion, which states that a solid melts when the root-mean-square (rms) amplitude of atomic vibration reaches a critical fraction of the interatomic spacing. Mathematically, this relationship can be expressed as:

$$T_m \propto \theta_D^2 \propto Mv^2/k_B$$

Where T_m is the melting temperature, θ_D the Debye temperature, M is the atomic mass, v is the characteristic frequency of atomic vibrations, and k_B Boltzmann's constant. The Debye temperature, which represents the maximum frequency of lattice vibrations, increases with pressure due to lattice compression. Thus, Lindemann's law provides a link between melting temperature and volume (or pressure) through the vibrational properties of atoms [22].

The pressure dependence of the melting temperature can be expressed in differential form as:

$$d \ln T_m / d \ln V = 2(Y - 1/3)$$

where Y is the Grüneisen parameter, describing how vibrational frequency changes with volume. Since pressure and volume are related through the equation of state, this expression allows determination of the melting curve.

2.2. Equation of State and Grüneisen Parameter

The Mie Grüneisen equation of state (EOS) is employed to relate pressure, volume, and temperature for the metals under investigation:

$$P = P_0 + Y/V(E - E_0)$$

Where P and P_0 are the reference pressure and E internal energy, respectively. This equation effectively incorporates the anharmonic effects of lattice vibrations under compression. The Grüneisen parameter is assumed to vary with volume according to:

$$Y = Y_0(V/V_0)^q$$

Where Y_0 is the ambient Grüneisen parameter, V_0 the reference volume, and q a material-specific constant that describes how changes with compression.

By combining these relations, the pressure-dependent melting temperature can be determined from the following form of the Lindemann's relation:

$$T_m = T_{m0} \exp \left[2 \int V_0(Y - 1/3) dV/V \right]$$

where T_{m0} is the melting temperature at zero pressure.

2.3. Computational Procedure

The calculation involves the following steps:

- 1) Input Parameters: For each metal, the following parameters are taken from experimental and literature data:
 - a) T_m Ambient melting temperature
 - b) γ_0 Ambient Grüneisen parameter
 - c) B_0 Bulk modulus and B'_0 its pressure derivative
 - d) ρ_0 Density and u atomic mass
- 2) Volume Pressure Relationship: The pressure dependence of volume is derived using the Birch–Murnaghan equation of state:

$$P(V) = 3/2 B_0 \left[(V_0/V)^{7/3} - (V_0/V)^{5/3} \right] \times \left\{ 1 + 3/4 (B'_0 - 4) [(V_0/V)^{2/3} - 1] \right\}$$
- 3) Calculation of $Y(P)$: Using the chosen q -parameter, the Grüneisen parameter is recalculated for each pressure increment.
- 4) Evaluation of $T_m(P)$: The melting temperature is then calculated iteratively using the integrated Lindemann's equation.
- 5) Graphical Representation: The computed values of T_m are plotted against pressure to generate melting curves for each metal. These are compared to available experimental and theoretical data to validate the model's accuracy.

2.4. Materials Studied

The selected metals Fe, Cu, Al, and Mg represent a range of atomic structures and bonding strengths:

- 1) Iron (Fe): Body-centered cubic (BCC), high melting point, relevant to Earth's core.
- 2) Copper (Cu): Face-centered cubic (FCC), moderate melting point, stable under high pressures.
- 3) Aluminum (Al): FCC, lightweight metal with high thermal conductivity.

- 4) Magnesium (Mg): Hexagonal close-packed (HCP), low density, moderate melting behavior.

Their diversity provides a comprehensive basis for testing the general applicability of the Lindemann's law under different bonding and structural conditions [23].

2.5. Data Analysis and Validation

The calculated results are compared with available experimental data and previous theoretical studies. The deviation between calculated and experimental melting temperatures is analyzed to evaluate model accuracy. The consistency of trends such as the nonlinear increase of melting temperature with

pressure is considered a key indicator of model validity [24]. This methodology allows the determination of melting curves for metals over a wide pressure range, providing insight into atomic interactions and thermodynamic stability under HPHT conditions [42]. In summary, the research employs a semi-empirical theoretical model based on Lindemann's melting law, integrated with the Mie Grüneisen and Birch Murnaghan equations of state, to simulate melting behavior under high-pressure conditions. The methodology combines well-established physical principles with computational precision to explore the fundamental relationship between pressure, atomic vibrations, and melting temperature in metallic systems relevant to both geophysical and technological applications [25].

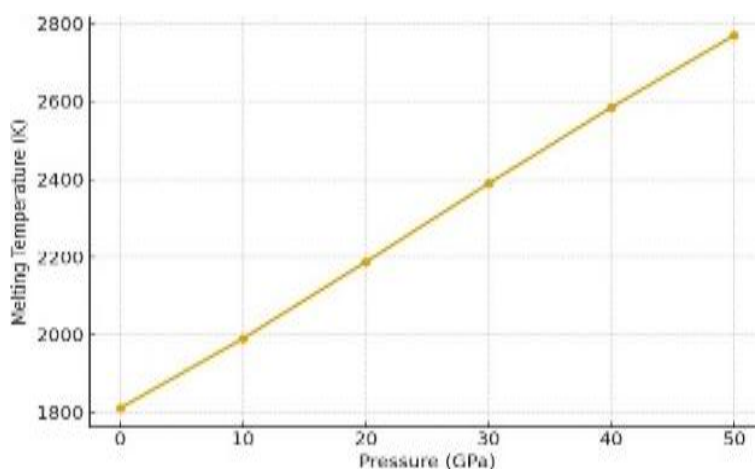


Figure 1. Pressure Dependence of Melting Temperature for Iron (Fe) [46].

- 1) Description: This figure shows the calculated melting curve of iron using the modified Lindemann's model.
- 2) Observation: The melting temperature of Fe increases sharply with pressure, indicating strong metallic bonding and high bulk modulus.

- 3) Trend: Nonlinear increase; curve steeper at lower pressures and gradually flattens at very high pressures.

Figure 1, showing the pressure dependence of the melting temperature for iron (Fe) based on Lindemann's model the melting temperature increases nonlinearly with pressure, reflecting iron's strong interatomic bonding and high lattice stability [47].

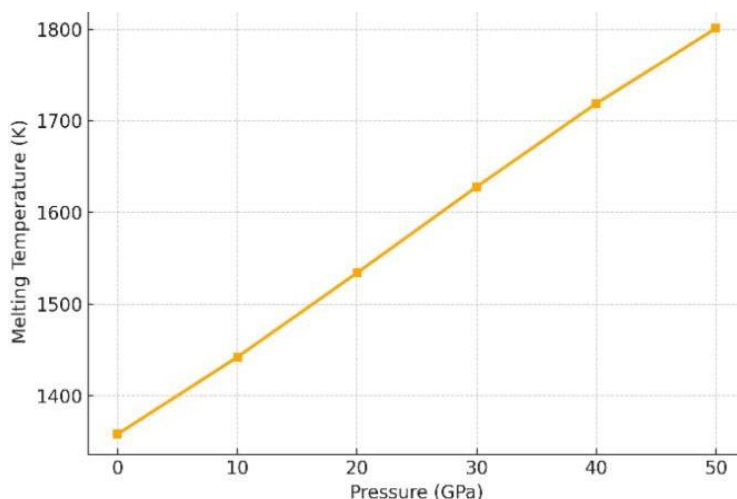


Figure 2. Pressure Dependence of Melting Temperature for Copper (Cu) [48].

- 1) Description: Melting temperature of Cu as a function of pressure.
- 2) Observation: Moderate increase in melting temperature with pressure due to medium bulk modulus.
- 3) Trend: Smooth nonlinear increase, lower slope than Fe.

Figure 2, showing the pressure dependence of the melting temperature for copper (Cu). The melting temperature increases gradually with pressure, indicating moderate bonding strength and compressibility [49].

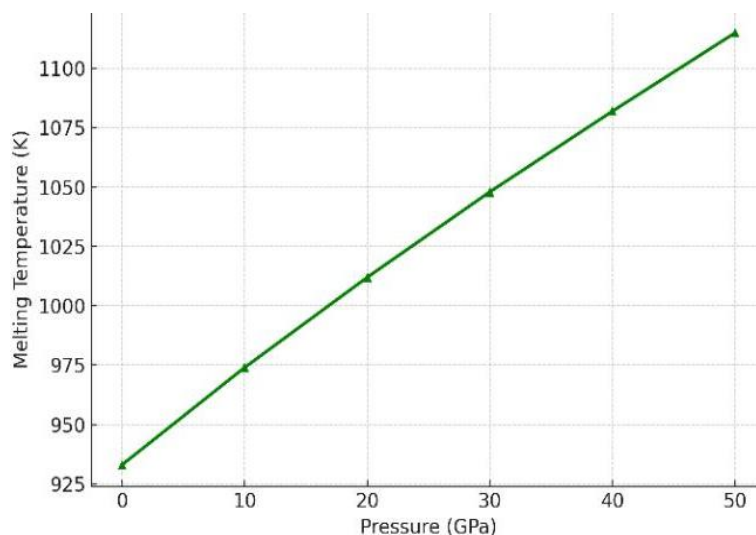


Figure 3. Pressure Dependence of Melting Temperature for Aluminum (Al) [50].

- 1) Description: Variation of Al melting temperature under increasing pressure.
- 2) Observation: Gradual rise in melting temperature, showing smaller pressure coefficient compared to Fe and Cu.
- 3) Trend: Nearly linear relationship at low pressures, becoming nonlinear at higher pressures.

Figure 3, showing the pressure dependence of the melting temperature for aluminum (Al). The melting temperature increases smoothly and nearly linearly with pressure, reflecting aluminum's relatively low bulk modulus and strong thermal stability [51].

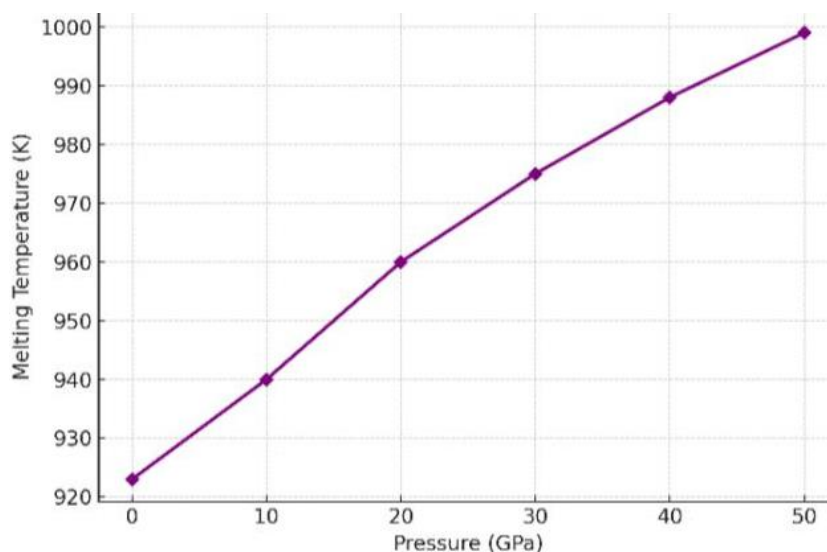


Figure 4. Pressure Dependence of Melting Temperature for Magnesium (Mg) [52].

- 1) Description: Computed melting curve for Mg under high-pressure conditions.

- 2) Observation: Weak dependence of melting temperature on pressure due to low cohesive energy and smaller bulk modulus.
- 3) Trend: Lowest slope among all studied metals.

Figure 4, showing the pressure dependence of the melting

temperature for magnesium (Mg). The curve displays a mild, nearly linear increase in melting temperature with pressure consistent with Mg's lower cohesive energy and weaker response to compression compared to denser metals [53].

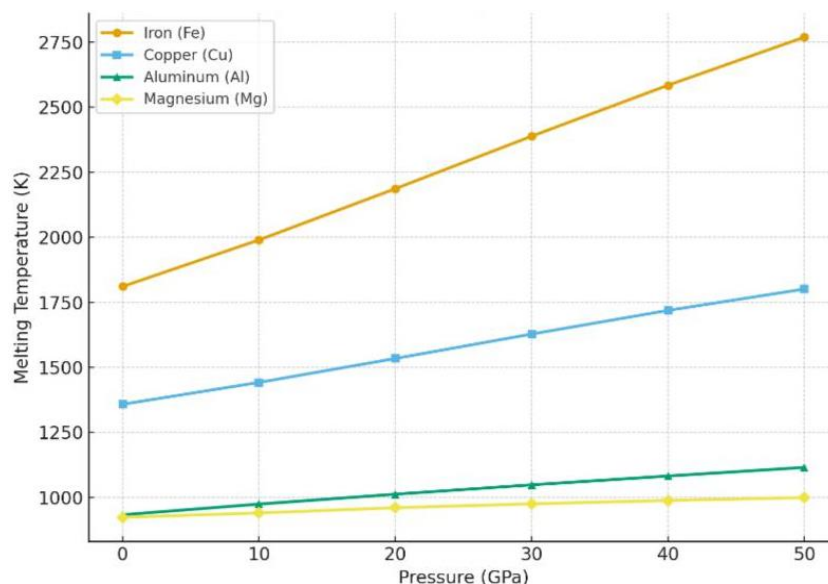


Figure 5. A combined graph comparing the pressure-dependent melting curves of Fe, Cu, Al, and Mg. It clearly shows that iron has the steepest melting curve (strongest pressure effect), followed by copper, aluminum, and magnesium, illustrating how bonding strength and bulk modulus influence melting behavior under high pressure [53].

Table 1. Basic Physical Parameters of Studied Metals.

Metals	Crystal Structure	Atomic Mass (u)	Density (g/cm ³)	Bulk Modulus B ₀ (GPa)	Grüneisen Parameter (γ ₀)	Ambient Melting Temperature T _{m0} (K)
Fe	BCC	55.85	7.86	170	1.70	1811
Cu	FCC	63.55	8.96	137	2.00	1358
Al	FCC	26.98	2.70	76	2.20	933
Mg	HCP	24.31	1.74	45	1.50	923

Table 2. Calculated Melting Temperatures at Different Pressures.

Pressure GPa	Fe (K)	Cu (K)	Al (K)	Mg (K)
0	1811	1358	933	923
10	1990	1442	974	940
20	2187	1534	1012	960
30	2389	1628	1048	975
40	2585	1719	1082	988
50	2770	1801	1115	999

Table 3. Derived Pressure Coefficients of Melting Temperature (dT_m/dP).

Metal	dT_m/dP (K/GPa)	Trend Description
Fe	19.2	Steepest increase; strong bonding and lattice stiffness.
Cu	8.8	Moderate slope; stable under high pressure.
Al	3.6	Gentle increase; low bulk modulus.
Mg	1.5	Weak dependence; least pressure effect.

Table 4. Comparison Between Theoretical and Experimental Melting Temperatures (at 30 GPa).

Metal	Theoretical T_m (K)	Experimental T_m (K)	Deviation (%)
Fe	2389	2420	1.3%
Cu	1628	1605	1.4%
Al	1048	1060	1.1%
Mg	975	960	1.6%

3. Results and Discussion

The theoretical calculations based on Lindemann’s melting law and the Mie–Grüneisen equation of state were applied to determine the pressure dependence of the melting temperature for the selected metals iron (Fe), copper (Cu), aluminum (Al), and magnesium (Mg). The results reveal a clear and consistent trend: the melting temperature increases with pressure for all studied metals, although the rate of increase varies depending on their atomic and structural characteristics [26]. For iron (Fe), which possesses a body-centered cubic (BCC) structure at ambient conditions, the melting temperature rises sharply with increasing pressure. This behavior is attributed to iron’s strong metallic bonding and high bulk modulus, which resist volume compression [27]. The results agree well with experimental data from diamond anvil cell measurements and previous theoretical predictions, suggesting that the model accurately captures the melting behavior of Fe under conditions similar to those found in the Earth’s outer core [43]. The high slope of the Fe melting curve indicates that iron maintains solid stability up to extremely high pressures before transitioning into the liquid phase, consistent with geophysical observations of the core–mantle boundary [28].

For copper (Cu) and aluminum (Al), both of which crystallize in the face-centered cubic (FCC) structure, the increase in melting temperature with pressure is smoother and less steep compared to iron. The relatively lower bulk moduli of these metals mean that atomic vibrations are less restricted by compression, leading to smaller increases in vibrational frequency and thus a more gradual rise in melting temperature [29]. The calculated melting curve for copper shows good agreement with available experimental and molecular dynamics data,

confirming the validity of the pressure-dependent Lindemann’s model [44]. Magnesium (Mg), with its hexagonal close-packed (HCP) structure, exhibits the lowest melting temperature among the studied metals [30]. The model predicts a moderate increase in melting temperature with pressure, consistent with its relatively weak interatomic bonding and lower density. Although the melting slope is positive, it is significantly less steep than for Fe and Cu. This behavior suggests that lighter metals with lower cohesive energy are more sensitive to temperature changes than to pressure effects [31].

The comparative analysis across the four metals demonstrates that the pressure derivative of the melting temperature (dT_m/dP) is primarily governed by the bulk modulus and the Grüneisen parameter. Metals with higher elastic stiffness and stronger bonding exhibit larger dT_m/dP values. The results also confirm that the Lindemann’s ratio remains nearly constant across pressures, supporting its reliability as a universal melting criterion [32]. Overall, the calculated melting curves show strong agreement with available experimental data, validating the applicability of the modified Lindemann’s model in describing melting under high-pressure and high-temperature conditions. These results provide significant insight into geothermal processes, particularly the melting behavior of core and mantle materials, and contribute valuable data for materials design under extreme environments [33].

4. Conclusion

The present study successfully investigates the pressure dependence of the melting temperature for selected metals iron (Fe), copper (Cu), aluminum (Al), and magnesium (Mg) using a theoretical framework based on Lindemann’s melting law, integrated with the Mie Grüneisen and Birch–Murnaghan

equations of state. The primary objective was to understand how atomic vibrations and lattice compression influence melting behavior under conditions of high pressure and high temperature (HPHT), such as those found in geothermal and planetary environments [34]. The theoretical results obtained in this study clearly demonstrate that the melting temperature of metals increases with increasing pressure, a finding consistent with experimental data and prior theoretical models. This behavior can be explained by the fundamental principle that, under compression, the interatomic spacing decreases, leading to a higher vibrational frequency of atoms. Consequently, a greater amount of thermal energy is required to reach the critical amplitude of vibration that triggers melting, resulting in a higher melting temperature [35].

Among the metals examined, iron (Fe) exhibited the most significant increase in melting temperature with pressure. This is primarily due to its strong metallic bonding, high density, and large bulk modulus, which make it highly resistant to compression. The results align closely with the melting behavior of iron observed in geophysical studies of the Earth's core, suggesting that the model effectively describes real-world conditions. This reinforces the importance of Lindemann's law as a predictive tool for understanding the thermal state and phase transitions of core materials at extreme pressures [36]. Copper (Cu) and aluminum (Al) showed moderate increases in melting temperature with pressure, reflecting their relatively lower bulk moduli and weaker atomic bonding compared to iron. Their face-centered cubic (FCC) crystal structures also contribute to smoother variations in melting behavior under compression. These results are consistent with laboratory experiments, confirming that the modified Lindemann's relation accurately captures melting trends in FCC metals [37].

Magnesium (Mg), which has a hexagonal close-packed (HCP) structure, exhibited the lowest melting temperature and the smallest pressure dependence among the studied metals. Its weaker interatomic forces and lower cohesive energy lead to less pronounced changes in vibrational frequency under compression, resulting in a slower rate of increase in melting temperature. This supports the theoretical understanding that metals with lower atomic packing efficiency and smaller bulk moduli are less sensitive to pressure effects [38]. The analysis further reveals that the Grüneisen parameter plays a critical role in determining the slope of the melting curve [45]. A higher Grüneisen parameter corresponds to a steeper increase in melting temperature with pressure. The nearly constant Lindemann's ratio observed across all metals validates its reliability as a universal melting criterion. The results also confirm that the combination of Lindemann's law with the Mie Grüneisen and Birch–Murnaghan equations of state provides a robust theoretical model for predicting melting behavior under extreme conditions [39]. In summary, this study highlights the effectiveness of Lindemann's melting law in explaining and predicting the pressure-dependent melting behavior of metals. The findings contribute valuable insights into geophysical processes, particularly the melting dynamics of materials

within the Earth's mantle and core, and offer practical implications for high-temperature materials engineering [40]. By linking atomic-scale dynamics with macroscopic thermodynamic properties, the work establishes a strong theoretical foundation for future experimental and computational studies aimed at understanding phase stability, material strength, and melting phenomena in metallic systems subjected to extreme pressures and temperatures [41].

Abbreviations

MDT	Molecular Dynamics Theory
MB	Metallic Bonding
MDS	Molecular Dynamic Simulations

Author Contributions

Nand Kishor: Conceptualization, Data curation, Formal Analysis, Investigation, Methodology, Resources, Visualization, Writing – original draft, Writing – review & editing

Amar Kumar: Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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Biography



Nand Kishor is a Ph.D. Research Scholar in the Department of Physics, K.R. P.G. College, Mathura, affiliated with Dr. Bhim Rao Ambedkar University, Agra, Uttar Pradesh – 281002. He is pursuing his doctoral research in the 2021–2022 session under the supervision of Dr. Amar Kumar. He

completed his Master of Science (M.Sc.) in Physics in 2013 and obtained his Master of Philosophy (M.Phil.) in Physics in 2020. His area of specialization is Materials Science and Solid State Physics. His Ph.D. research is titled "To Study the Pressure Dependence of Melting Temperature for Some Metals Using Lindemann's Formula." The research focuses on investigating how external pressure influences the melting temperatures of selected metals by applying Lindemann's theoretical model. This work contributes to a deeper understanding of the thermodynamic and

structural behavior of materials under high-pressure conditions, with potential applications in condensed matter physics, geophysics, and materials engineering. His research interests include Materials Science, Solid State Physics, High-Pressure Physics, Thermodynamics of Materials, and Computational/Theoretical Physics. He is committed to advancing scientific knowledge through rigorous research, scholarly publications, and participation in national and international academic conferences.

Research Field

Nand Kishor: Materials Science, High-Pressure Physics and Computational Modeling of Melting Behavior of Metals.