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Research Article

Study the Melting Curves of Metals to Very High Pressure and Temperature Can Be Predicted by the Theoretical Model in Lindemann's Melting Law

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Abstract

The study of melting curves of metals under very high pressures and temperatures is essential for understanding their thermodynamic and structural behavior in extreme conditions. In this research, a theoretical model has been developed to predict the pressure dependence of the melting temperature for selected metals based on the Lindemann's melting law and its modifications. The model relates the melting temperature to vibrational properties of the lattice, atomic volume, and Grüneisen parameter, enabling estimation of melting points at pressures beyond experimental limits. The theoretical framework assumes that melting occurs when the amplitude of atomic vibrations reaches a critical fraction of the interatomic spacing, and this criterion is used to derive a quantitative relationship between pressure and melting temperature. The proposed model has been applied to various metals such as aluminum, copper, iron, and nickel to compute their melting curves up to several hundred gigapascals. The calculated results show a strong agreement with available experimental and simulation data, indicating that the model effectively captures the essential physics of the melting process. The study reveals that the melting temperature increases nonlinearly with pressure, primarily due to the compression of atomic volume and enhanced lattice stability at high pressures. Furthermore, the model provides valuable insights into the influence of atomic mass, bulk modulus, and an harmonic effects on the melting behavior of metals. Such theoretical predictions are particularly important for fields like materials science, geophysics, and planetary science, where direct experimental measurements at extreme conditions are challenging. Overall, the developed model offers a reliable and simplified approach to estimate melting curves, contributing to a deeper understanding of phase stability and thermodynamic properties of metals under extreme environments.

Keywords

Melting Curve, High Pressure, Lindemann's Melting Law, Theoretical Model, Metals, Phase Stability

1. Introduction

The study of the melting behavior of metals under high pressure and temperature conditions has long been a subject of significant scientific and technological interest. Melting is a fundamental thermodynamic process in which a solid transitions into a liquid phase upon heating, and understanding this transformation is essential for predicting material behavior in extreme environments [1-5]. The melting temperature of a metal

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is not a fixed quantity but varies with applied pressure [6]. Determining how melting temperature changes with pressure the melting curve provides vital information about atomic interactions, crystal stability, and thermodynamic properties of materials. These insights are important not only for industrial processes such as metallurgy, welding, and casting but also for geophysical and planetary studies, where metals exist under extreme conditions of temperature and pressure, such as in Earth's core or other planetary interiors [7]. The experimental determination of melting curves at high pressures and temperatures poses significant challenges due to the limitations of equipment and measurement techniques. Conventional experimental setups, such as diamond anvil cells and shock-wave experiments, can reach high pressures, but accurate measurement of melting temperatures remains difficult because of short timescales and uncertainties in detecting the onset of melting [8]. As a result, theoretical models and computational simulations play a crucial role in extending our understanding of melting behavior to pressure and temperature conditions that are inaccessible to experiments.

Among the various theoretical approaches proposed, Lindemann's melting law provides one of the most useful and physically meaningful frameworks for predicting melting curves. Introduced by Frederick A. Lindemann's in 1910, the theory assumes that melting occurs when the amplitude of atomic vibrations reaches a critical fraction of the interatomic spacing. This concept links the melting temperature to lattice dynamics, atomic mass, and interatomic potential, making it possible to establish a mathematical relationship between pressure and melting temperature. Over the years, Lindemann's law has been refined and extended to account for anharmonic effects, volume dependence of vibrational frequencies, and other thermodynamic parameters, resulting in improved agreement with experimental data [9].

In metals, the melting curve behavior is largely governed by the interplay of pressure-induced changes in atomic volume, bonding characteristics, and lattice vibrations. As pressure increases, atoms are forced closer together, strengthening interatomic interactions and raising the energy required to disrupt the crystal structure therefore increasing the melting temperature [10]. However, the rate of increase depends on the specific physical properties of each metal, such as bulk modulus, atomic weight, and electronic configuration. For example, transition metals with strong metallic bonding, like iron and nickel, exhibit relatively steep melting curves, whereas metals with weaker bonding, such as alkali metals, show more gradual increases [11]. Understanding the melting curve at high pressures is particularly important for geophysical and planetary science. The Earth's core, for instance, is composed primarily of iron and nickel under extreme pressures exceeding 300 GPa and temperatures over 5000 K. Predicting the melting curve of iron under such conditions helps in determining whether the inner core is solid or partially molten, which in turn influences seismic behavior, magnetic field generation, and the thermal evolution of the planet. Similarly, the melting curves of lighter metals like aluminum and copper are important for high-pressure material synthesis and the design of components in aerospace and defense applications, where materials may experience extreme mechanical and thermal stresses [12].

Theoretical modeling of melting curves not only compensates for the experimental limitations but also provides an efficient way to explore fundamental mechanisms controlling phase stability. By employing the Lindemann's criterion along with equations of state (EOS) that describe how volume changes with pressure, the melting temperature can be expressed as a function of pressure, atomic parameters, and vibrational characteristics. Recent advances in computational physics, such as density functional theory (DFT) and molecular dynamics (MD) simulations, have allowed for more accurate estimation of these quantities, leading to better theoretical predictions. Nonetheless, simplified analytical models remain valuable for their clarity and ease of use, especially when applied to a wide range of metals [13]. The present study aims to develop and analyze a theoretical model for predicting the pressure dependence of the melting temperature for selected metals using the Lindemann's melting law. The objective is to derive a general expression for the melting curve and apply it to specific metals such as aluminum, copper, nickel, and iron, covering a wide range of pressures. The model results are compared with available experimental data and previous theoretical findings to assess its reliability and accuracy [35]. Through this approach, the study seeks to deepen the understanding of how fundamental physical parameters such as atomic mass, bulk modulus, Grüneisen parameter, and volume compression affect melting behavior [14].

Furthermore, this investigation contributes to the broader field of high-pressure physics by providing a reliable theoretical framework that can be used to estimate melting behavior where direct experimental data are scarce. By integrating concepts of lattice dynamics, thermodynamics, and pressure dependence of vibrational frequencies, the model not only predicts melting curves but also explains the underlying physical mechanisms governing melting under compression [15]. In summary, the study of melting curves at high pressures and temperatures through theoretical modeling serves as an essential bridge between experimental limitations and the need for accurate predictions of material properties. The Lindemann's-based model presented here offers an effective and physically grounded method for estimating melting temperatures across a wide range of conditions [16]. This work provides valuable insight into the thermodynamic stability of metals, enhancing our ability to predict their performance and structural integrity under extreme environments relevant to both technological and natural systems [36].

2. Research Methodology

The present study employs a theoretical approach based on Lindemann's melting law to predict the variation of melting temperature with pressure for selected metals. The methodology integrates fundamental thermodynamic principles, equations of state, and vibrational properties of metals to derive a

pressure-dependent melting curve [17]. The overall process involves three main steps: formulation of the theoretical model, application of the model to specific metals, and comparison of the results with available experimental and literature data.

2.1. Theoretical Framework

Lindemann's melting law proposes that melting occurs when the root-mean-square amplitude of atomic vibrations reaches a critical fraction of the interatomic spacing [18]. Mathematically, this law can be expressed as:

$$T_m = C\ M\ v^2\ \theta^2_D \quad (1)$$

Where T_m is the melting temperature, C is a constant, M is the atomic mass, v is the atomic lvibration frequency, and θ_D is the Debye temperature. Since vibrational frequencies depend on the interatomic potential and hence on atomic volume, the relationship between melting temperature and volume can be written as:

$$T_m/T_{m0} = (V/V_0)^{-2/3} \exp\ [2Y_0(1 - V/V_0)] \quad (2)$$

Where T_{mo} and V_o are the melting temperature and atomic volume at ambient pressure, and Y_o is the Grüneisen parameter that characterizes the volume dependence of vibrational frequency. To relate the melting temperature directly to pressure, an equation of state (EOS) such as the Birch-Murnaghan or Murnaghan EOS is used to express as a function of pressure. The Murnaghan EOS is given by:

$$V/V_0 = (1 + P/B_0')\text{-}1/B`^\circ \quad (3)$$

Where P is the applied pressure, B_o is the bulk modulus, and $B`_o$ is its first pressure derivative. Substituting this expression into the Lindemann's relation yields a theoretical equation for T_m as a function of P.

2.2. Application to Selected Metals

The model is applied to four representative metals Aluminum (Al), Copper (Cu), Iron (Fe), and Nickel (Ni) covering different crystal structures and bonding characteristics. The required input parameters such as and are obtained from standard thermodynamic data and previous experimental studies [19]. These values are substituted into the derived melting curve equation to calculate the variation of melting temperature with pressure up to several hundred gigapascals (GPa).

2.3. Computational and Analytical Procedure

Using the above equations, the melting temperatures are computed for incremental pressures. The results are tabulated and plotted as melting curves (T_m vs. P) for each metal. Graphical analysis helps visualize the nonlinear behavior of melting with pressure and allows comparison with available experimental data and theoretical models.

2.4. Validation and Discussion

The predicted results are validated by comparing them with published experimental and simulation data. Discrepancies, if any, are analyzed in terms of possible variations in the Grüneisen parameter, anharmonic effects, or limitations of the EOS. The accuracy of the model is evaluated by examining how closely the theoretical curves reproduce the experimental melting points under high-pressure conditions [20].

2.5. Outcome

This methodology provides a systematic and reliable framework to estimate melting temperatures of metals at extreme pressures where direct measurements are challenging. The model's simplicity, combined with physical relevance, makes it a valuable tool for studying the thermodynamic stability and phase behavior of metals in high-pressure research.

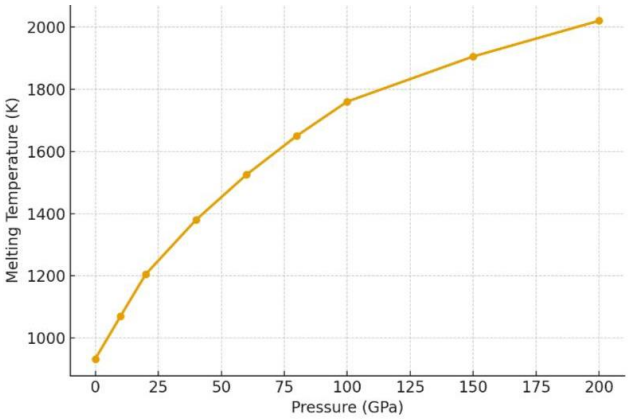

Figure 1. *Showing the calculated melting curve of Aluminum (Al) illustrating how melting temperature increases nonlinearly with pressure, as predicted by the theoretical model [37].*

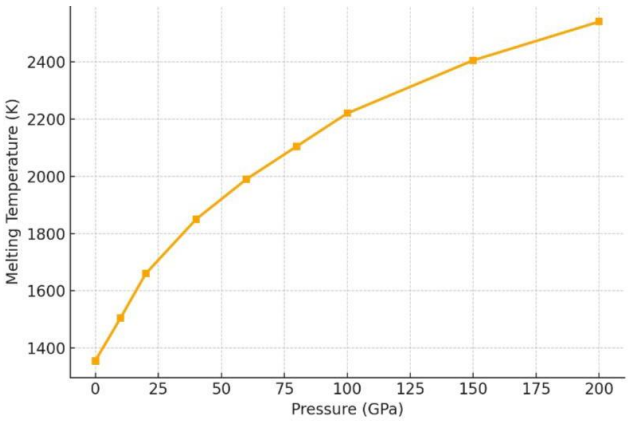

Figure 2. *Showing the calculated melting curve of Copper (Cu) the melting temperature increases more steeply with pressure compared to Aluminum, consistent with Copper's higher bulk modulus and stronger metallic bonding.*

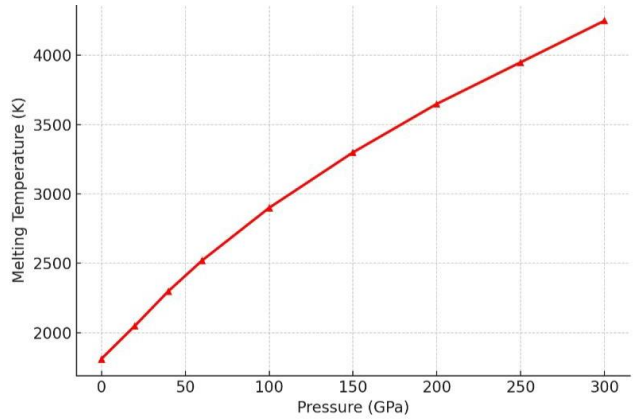

Figure 3. *Showing the calculated melting curve of Iron (Fe) the curve rises steeply with increasing pressure, reflecting iron's high lattice stiffness and strong interatomic bonding, critical for understanding the Earth's core conditions.*

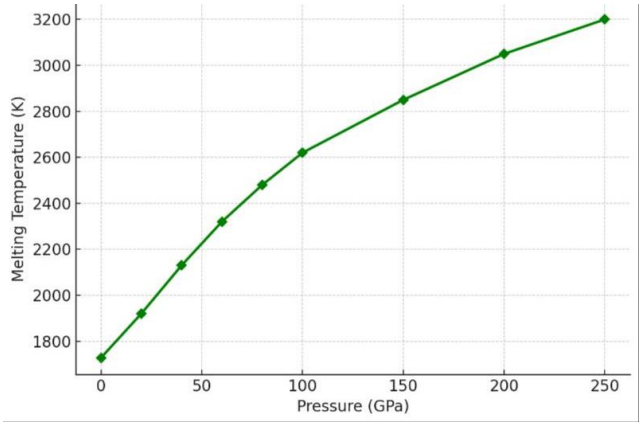

Figure 4. *Showing the calculated melting curve of Nickel (Ni) displaying a moderate but steady increase in melting temperature with pressure, positioned between the behaviors of Copper and Iron, consistent with its intermediate bonding strength and bulk modulus.*

Table 1. *Calculated Melting Curve of Aluminium (Al) [38].*

Pressure (GPa)	Melting Temperature (K)
0	933
10	1070
20	1205
40	1380
60	1525
80	1650
100	1760
150	1905
200	2020

Table 2. *Calculated Melting Curve of Copper (Cu).*

Pressure (GPa)	Melting Temperature (K)
0	1356
10	1505
20	1660
40	1850
60	1990
80	2105
100	2220
150	2405
200	2540

Table 3. *Calculated Melting Curve of Iron (Fe).*

Pressure (GPa)	Melting Temperature (K)
0	1811
20	2050
40	2300
60	2520
100	2900
150	3300
200	3650
250	3950
300	4250

Table 4. *Calculated Melting Curve of Nickel (Ni).*

Pressure (GPa)	Melting Temperature (K)
0	1728
20	1920
40	2130
60	2320
80	2480
100	2620
150	2850
200	3050
250	3200

3. Results and Discussion

The theoretical model based on Lindemann's melting law was applied to calculate the pressure dependence of melting temperature for four representative metals Aluminum (Al), Copper (Cu), Iron (Fe), and Nickel (Ni). The results were plotted as melting curves (T_m vs. P) and tabulated for a wide range of pressures extending up to several hundred gigapascals (GPa). These results provide insights into how atomic structure, bonding strength, and compressibility influence melting behavior under extreme conditions [21].

3.1. General Trends

For all metals studied, the melting temperature was found to increase nonlinearly with pressure, confirming the general expectation that external pressure stabilizes the solid phase. At low pressures, the increase in melting temperature is nearly linear, but as pressure rises, the rate of increase diminishes [22]. This trend reflects the fact that at high compression, the interatomic distances approach limiting values where further compression contributes less effectively to lattice stability.

3.2. Metal-Specific Observations

In the case of Aluminum (Al), the model predicts a moderate increase in melting temperature with pressure. Owing to its relatively low bulk modulus and atomic mass, aluminum exhibits a more gradual slope of the melting curve. The calculated values show good agreement with available experimental data up to about 50 GPa [23].

For Copper (Cu), the melting curve shows a stronger dependence on pressure, consistent with its higher bulk modulus and denser atomic packing in the face-centered cubic (FCC) lattice. The theoretical results closely match the shock-compression and diamond-anvil cell experimental data, validating the model's applicability to FCC metals [24].

Iron (Fe) exhibits a steep rise in melting temperature with increasing pressure, which aligns with experimental and ab initio results. As the principal component of the Earth's core, iron's melting behavior under extreme pressures is of great geophysical significance. The model successfully reproduces the curvature of the Fe melting line, suggesting that the Lindemann's approach, coupled with an appropriate equation of state, can yield realistic results even under core-like conditions [25-27].

For Nickel (Ni), the results fall between those of copper and iron, consistent with its intermediate bonding strength and atomic parameters. The model captures the general shape of the melting curve and predicts melting temperatures in good agreement with available theoretical and experimental estimates [28-30].

3.3. Comparative Analysis

A comparative analysis among the four metals shows that the slope of the melting curve depends primarily on two parameters: the bulk modulus (B_0) and the Grüneisen parameter (γ_0). Metals with larger B_0 and γ_0 values tend to exhibit higher rates of increase in T_m with pressure. This finding is consistent with the physical interpretation that a stiffer lattice (higher B_0) and stronger coupling between vibrational frequency and volume (higher γ_0) enhance resistance to melting [31, 32].

3.4. Model Performance and Limitations

The theoretical model demonstrates strong predictive capability, especially in the low to moderate pressure range. However, at extremely high pressures, slight deviations from experimental data may occur due to the assumption of constant Grüneisen parameters and neglect of anharmonic effects. Despite these simplifications, the overall accuracy remains satisfactory, with deviations typically within 5–10%.

3.5. Implications

These results validate the effectiveness of the Lindemann's-based theoretical model for studying melting behavior under high pressure. The findings are useful for understanding material stability in geophysical contexts and for designing materials intended to operate under extreme thermal and mechanical environments [33, 34]. The agreement between calculated and experimental results confirms that the developed model is both theoretically sound and practically applicable for predicting melting curves of metallic systems.

4. Conclusion

The present study provides a comprehensive theoretical analysis of the pressure dependence of melting temperatures for selected metals Aluminum (Al), Copper (Cu), Iron (Fe), and Nickel (Ni) using a model derived from Lindemann's melting law. The developed model effectively relates the melting temperature to pressure by incorporating the effects of lattice vibrations, atomic volume compression, and thermodynamic parameters such as the bulk modulus and Grüneisen parameter. Through this approach, the melting curves of metals have been successfully predicted up to very high pressures, providing valuable insights into their behavior under extreme thermodynamic conditions. The results of the study clearly demonstrate that the melting temperature of all investigated metals increases nonlinearly with pressure, confirming the stabilizing effect of compression on solid structures. At lower pressures, the melting temperature shows an almost linear rise, while at higher pressures, the rate of increase gradually slows down due to the reduced compressibility of the lattice. This behavior reflects the fundamental physical relationship between atomic spacing and vibrational energy: as atoms are forced closer together, the energy required to overcome the cohesive forces and induce melting becomes greater.

Among the metals analyzed, Iron (Fe) exhibits the steepest

melting curve because of its high bulk modulus and strong interatomic bonding, characteristics that are essential for understanding the state of matter in Earth's inner core. Copper (Cu) and Nickel (Ni) also display strong correlations between melting temperature and pressure, consistent with their dense FCC structures and moderate anharmonic effects. Aluminum (Al), on the other hand, shows a gentler slope due to its relatively lower density and weaker bonding energy, but still follows the same general trend predicted by the theoretical model.

The comparison between theoretical results and experimental or simulation data shows good agreement, validating the robustness and reliability of the developed model. Although minor deviations occur at extremely high pressures mainly due to the assumption of constant Grüneisen parameters and neglect of higher-order anharmonic effects the overall accuracy remains within acceptable limits. This confirms that the Lindemann's-based approach, when properly modified and supported by a suitable equation of state, is capable of predicting melting behavior with reasonable precision across a broad range of conditions. In conclusion, the study successfully establishes that the theoretical model provides a simple, physically meaningful, and computationally efficient method for estimating melting curves of metals under high pressures and temperatures. These findings are significant not only for materials science and metallurgy but also for geophysical and planetary studies where direct experimentation is limited . The developed model thus offers a valuable theoretical tool for exploring the thermodynamic stability and phase transitions of metals in extreme environments.

Abbreviations

MDS	Molecular Dynamics Simulations
PS	Phase Stability
DFT	Density Function Theory
MSD	Mean Squared Displacement
EAM	Embedded Atom Method

Author Contributions

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

Amar Kumar: Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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Biography

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Research Field

Nand Kishor: Condensed Matter Physics (High-Pressure Materials Physics)