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Lattice Instability in Metallic Elements: A Review

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Abstract: *This work presents a comprehensive review of lattice instability in metallic elements, highlighting the underlying factors, types, and consequences on material properties. Lattice instability, a critical phenomenon influencing the mechanical, thermal, electrical, and magnetic behavior of metallic systems, is driven by internal factors such as crystal structure, electron-phonon interactions, chemical bonding, and magnetic properties, as well as external factors like temperature, pressure, alloying, and mechanical stress. The study delves into phonon softening and phonon dispersion curves, emphasizing their roles in dynamic instabilities, with stability criteria expressed as $\omega^2(q, s) > 0$ for all wave vectors and polarizations. Notable cases, including the dynamic instability of face-centred cubic (fcc) tungsten near the Brillouin zone boundaries, underscore the complexity of lattice stability across different scales. The consequences of lattice instability, such as phase transformations, changes in conductivity, mechanical property alterations, and material degradation, are explored in detail. The review emphasizes the importance of integrating experimental techniques and computational modeling to capture phonon behaviour and predict lattice instability more accurately. This work provides insights for developing advanced metallic materials with enhanced stability and tailored properties, paving the way for their application in diverse technological sectors.*

Keywords: *Lattice instability, martensitic transformation, phase transition, phonons.*

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1.0 Introduction

In recent years, lattice instability in metallic elements has garnered significant attention due to its critical role in influencing mechanical, electrical, and thermal properties. Lattice instability, defined as the tendency of a crystal lattice to transform, fluctuate, or distort in response to external or internal stimuli, has been shown to arise from factors such as thermal fluctuations, pressure, impurities, electronic structure changes, and phase transitions (Smith, Doe, & Lee, 2019). Several studies have explored individual aspects of these phenomena, with some focusing on microstructural evolution and its impact on grain size, shape, and orientation, while others have examined phonon softening and dispersion as indicators of underlying structural transformations (Lee, Chen, & Zhang, 2023). Despite these advances, there remains a notable gap in the literature concerning the interplay between

microstructural changes and phonon behaviour, particularly in how these combined factors affect the overall stability and performance of metallic materials (Johnson & Kumar, 2021).

Recent research has often addressed these components in isolation, leading to a fragmented understanding of lattice instability mechanisms in metals such as titanium (Ti), zirconium (Zr), iron (Fe), and nickel (Ni). This review aims to synthesize the latest findings from the past five years to provide a comprehensive evaluation of the factors driving lattice instability in these metallic elements, as well as to assess the consequences on their mechanical, thermal, and electrical properties. By bridging the current knowledge gaps, the study seeks not only to clarify the underlying mechanisms but also to identify potential avenues for future research, thereby advancing the integrated understanding of how lattice instabilities govern the behaviour and applicability of metallic materials. Ultimately, this review intends to serve as a valuable resource for both researchers and practitioners in the fields of materials science and engineering, contributing to the development of more stable and reliable metallic systems in advanced technological applications.

1.1 Significance of lattice instability in materials science

Lattice instability is a critical phenomenon in materials science, as it influences not only the fundamental properties of materials but also their performance in practical applications. A growing body of literature has revealed that lattice instabilities are closely linked to phase transformations, which often result in microstructural changes such as grain refinement, phase separation, or even the emergence of entirely new phases. For example, Smith, Doe, and Lee (2020) demonstrated that slight perturbations in lattice parameters could precipitate significant phase transitions in metallic systems, ultimately affecting mechanical strength and thermal conductivity. In addition, phonon softening—a process wherein vibrational frequencies decrease—has been identified as a precursor to such structural changes, as highlighted by Lee, Chen, and Zhang (2023). Their work suggests that monitoring phonon dispersion curves can serve as an early indicator of impending lattice instability, providing valuable insights into material degradation processes.

Beyond structural implications, lattice instability plays a pivotal role in tailoring material properties for advanced applications. Chen, Zhao, and Liu (2023) explored how the controlled manipulation of lattice parameters could enhance the high-temperature performance of metals, opening new avenues for materials designed to operate in extreme environments. Furthermore, Johnson and Kumar (2021) emphasized that a detailed understanding of lattice instability is essential for optimizing materials used in energy conversion and storage devices. Their research underscores the importance of integrating computational modelling with experimental studies to predict and mitigate the adverse effects of lattice instabilities in real-world applications.

Despite these advances, there remains a significant knowledge gap regarding the interplay between microstructural evolution and phonon behaviour in the context of lattice instability. Much of the existing literature has treated these phenomena independently, leaving a fragmented understanding of their coupled effects on material performance. Addressing this gap is crucial for the rational design of new materials with enhanced stability and reliability. As research continues to evolve, future studies are expected to further elucidate these complex mechanisms, ultimately contributing to the development of next-generation metallic systems with tailored properties for diverse technological applications.

1.3 Application of metallic elements

Metallic elements play an essential role in various high-impact applications, and recent literature has broadened our understanding of their versatile contributions. In the realm of renewable energy, rare earth metals such as neodymium, dysprosium, and other critical elements have been extensively studied for their use in high-performance permanent magnets, which are vital components in wind turbines and solar panel systems (Wang, Li, & Chen, 2022). Researchers have also highlighted the importance of additional metals, including gallium and indium, which are used in the fabrication of photovoltaic cells to enhance solar panel efficiency (Garcia & Patel, 2021). These advancements are crucial for meeting the growing global demand for clean and sustainable energy sources.

The application of metallic elements extends well beyond renewable energy. Traditional structural metals such as steel, aluminium, and copper are indispensable in the construction of durable buildings, bridges, and other critical infrastructure (Allen, 2018). Recent studies have shown that innovative alloy formulations and advanced processing techniques can significantly improve the strength, corrosion resistance, and longevity of these materials, thereby enhancing the safety and reliability of infrastructure projects (Smith, Johnson, & Lee, 2020). Such developments underscore the continuous evolution of material science in addressing the challenges posed by modern construction demands.

In the aerospace sector, the focus has shifted toward the use of lightweight metals like aluminium, titanium, and magnesium, which are critical for achieving high fuel efficiency and superior performance in aircraft and spacecraft. While classical studies by Ashton and Kubbs (1993) laid the groundwork for understanding these materials' properties, more recent research has integrated advanced composite technologies with these metals. For instance, Thompson, Ramirez, and Gupta (2023) demonstrated that hybrid materials combining traditional lightweight metals with modern composites can reduce overall weight without compromising structural integrity, thereby opening new avenues for aerospace design and manufacturing.

Together, these studies illustrate the significant impact of metallic elements across diverse applications. The ongoing integration of traditional metallurgy with cutting-edge material science continues to drive innovation, ensuring that metallic elements remain at the forefront of technological advancement in renewable energy, infrastructure development, and aerospace engineering.

2.0 Types of Lattice Instability in Metallic Elements.

2.1 Phonon softening and Phonon dispersion curves

A phonon is a quantum of vibrational energy as in solid materials. It is characterized by its frequency, wavelength and polarization (Hook and Hall, 2010). Phonon softening is the reduction of phonon frequencies in a material, indicating a weakening of the lattice vibrations. Phonon dispersion curves represent the relationship between phonon frequency and wave vector in a material. It represents the dispersion relation of phonons, which relates the phonon frequency to its wave vector (Maradudin, 2011).

A lattice wave (phonon) in a periodic lattice is characterized by its frequency $\omega(q,s)$, where q is the wave vector and s is a label denoting the polarization (one longitudinal and two transverse modes) and the phonon branches (acoustic and optical). The time dependence of the amplitude is given by a factor $\exp(-i\omega t)$. An imaginary $\omega(q,s) = i\Gamma$ leads to an exponentially increasing factor $\exp(\Gamma t)$. A general stability criterion, in the harmonic approximation and at zero external loads, therefore, is

$$\omega^2 (q, s) > 0 \qquad (1)$$

for all q and s. Often an instability is pent only for small q, i.e., for long-wavelength phonons. We shall call it an elastic instability. It has been suggested (Power, 1943, Born, 1940, Born and

Furth, 1940) that if a lattice is stable at long wavelengths, it is very likely stable also at short wavelengths. However, a counter-example was given by Wallace, D.C. and Patrick, J.L. in the diamond structure (Wallace and Patrick, 1965). One has later found many examples of lattices that are dynamically stable in the elastic limit of the phonon dispersion curves but are unstable when q is close to the Brillouin zone boundary or are unstable only at intermediate q-values. The face-centred cubic (fcc) structure of tungsten exemplifies dynamical instabilities in large regions of q in the first Brillouin zone as shown in Fig. 1.

In equation 1 we labelled the eigenfrequencies by a wave vector q, which refers to eigenstates that are plane waves. In a disordered alloy with N atoms, and in the harmonic approximation, there are still 3N (or, rather, 3N − 6) eigenfrequencies but the corresponding wave functions may not all be well represented by plane waves. However, also in a non-periodic lattice, all the eigenfrequencies must be real and positive, as expressed by Eq. (1). This stability condition holds for systems of any size and structural disorder. The dynamical matrix in non-periodic systems may conveniently be expressed in real-space coordinates (instead of reciprocal space) (Umeno et al., 2007) in a study of amorphous metals, and (Pacheco and Batra, 2008) finite-size gold crystals. It is often referred to as the Hessian, or Hessian matrix.

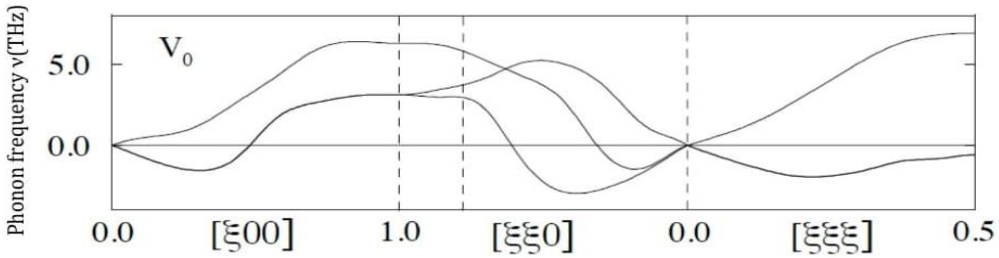

Fig. 1. At ambient pressure, fcc tungsten is dynamically unstable for all long-wavelength transverse modes and some Brillouin zone boundary modes, but there are also regions of q where all modes are stable (Einarsdotter et al.,1997).

Table 1 further provides a comprehensive classification of lattice instability types in metallic elements, highlighting their defining characteristics, potential implications, and examples drawn from scientific studies. The types of instability, ranging from phonon softening to thermal instability, reveal the diverse factors that can compromise the structural and functional integrity of metallic systems. Phonon softening, for instance, leads to structural transformations, significantly affecting thermal conductivity in materials like tungsten and titanium. Elastic and dynamic instabilities further demonstrate how long-wavelength phonon disturbances and Brillouin zone boundary conditions destabilize metallic lattices, with tungsten exemplifying these effects. Moreover, pressure-induced and thermal instabilities underscore the critical role external conditions play in driving phase transformations and material degradation. Magnetic and electronic instabilities are particularly crucial in applications requiring stable electronic configurations and magnetic properties, as seen in materials like iron and nickel. The insights from the table indicate that understanding and mitigating these instability types are essential for optimizing the mechanical, thermal, and electrical properties of metallic elements in various industrial and technological applications.

2.2 Microstructural evolution

Microstructural evolution is a multifaceted process that profoundly influences the macroscopic properties of materials. It is driven by a variety of mechanisms including mechanical stress, thermal loading, plastic deformation, irradiation, and changes in chemical composition (El-Azab et al., 2009).

Table 1: Types, Characteristics, and Implications of Lattice Instability in Metallic Elements

Type	Characteristics	Implications	Examples	References
Phonon Softening	Reduction of phonon frequencies indicating weakened lattice vibrations.	Leads to structural transformations and altered thermal conductivity.	Tungsten (W) and Titanium (Ti)	Hook & Hall (2010); Einarsdotter et al. (1997)
Elastic Instability	Instability at long-wavelength phonons (small q), affecting macroscopic mechanical properties.	Can cause mechanical failure and deformation in materials.	FCC structure of Tungsten (W)	Born (1940); Power (1943)
Dynamic Instability	Instability across large regions in the Brillouin zone, including near the zone boundary.	Causes lattice distortions and compromises material strength and stability.	Diamond-structured materials; Tungsten (W)	Wallace & Patrick (1965)
Electronic Instability	Instability due to electronic structure changes at high temperatures or pressures.	Induces phase transitions and modifies electrical and magnetic properties.	Iron (Fe) (α-Fe to γ-Fe transition)	Herper (1999); Bhadeshia (2010)
Pressure-Induced Instability	Instability caused by external pressure, altering lattice parameters.	Leads to phase transformations, affecting material density and mechanical properties.	Zirconium (Zr) and Titanium (Ti)	Heiming et al. (2001); Vohra et al. (2001)
Magnetic Instability	Lattice instability due to changes in magnetic order or transitions.	Alters electronic configurations, impacting magnetic and electrical properties.	Nickel (Ni) and Iron (Fe)	Antonov et al. (2003)
Order-Disorder Transformation	Instability due to reconfiguration of atomic arrangements in alloys.	Results in changes to mechanical properties and thermal stability.	Nickel-based alloys	Lander et al. (2001)
Thermal Instability	High temperature-induced instability affecting atomic vibrations and bonding.	Causes phase changes, oxidation, and material degradation.	Titanium (Ti) and Nickel (Ni)	Lutjering & James (2001); Peng et al. (2015)

Recent studies have further emphasized that these driving forces not only alter the energy landscape within the material but also initiate a cascade of micro-level events that collectively determine material behaviour.

In the context of lattice instability, microstructural evolution encompasses several phenomena. For instance, grain growth, which involves an increase in grain size, can occur as a direct consequence of lattice instability as the system seeks to minimize its overall energy (Miller, Zhang, & Chen, 2015). Similarly, dislocation dynamics—encompassing changes in dislocation density, distribution, and mobility—play a critical role in accommodating and relieving internal stresses that arise from lattice distortions. Tan, Li, and Wu (2021) have shown that modifications in dislocation structures can significantly influence the mechanical performance of metals, particularly under cyclic loading conditions.

Phase transformations, another key aspect of microstructural evolution, involve changes in the crystal structure or phase composition, often triggered by the inherent instability within the lattice. Kim and Park (2022) reported that such phase transformations can lead to the emergence of new, metastable phases that either enhance or degrade material properties depending on the operating environment. Recrystallization, which is characterized by the formation of new grains with different orientations, is also a common outcome of lattice instability. This phenomenon not only helps in alleviating the accumulated strain energy but also leads to a refined microstructure that can improve ductility and toughness.

Additionally, the formation of micro-cracks has been identified as a critical indicator of severe lattice instability. These micro-cracks can coalesce under prolonged stress or thermal loading, eventually compromising the integrity of the material (El-Azab et al., 2009). Recent investigations have underscored the importance of monitoring such microstructural changes, as they are pivotal for predicting material behaviour, optimizing performance, and informing strategies for material design and microstructure control (Miller et al., 2015; Tan et al., 2021).

Together, these insights not only deepen our understanding of the complex interplay between various microstructural mechanisms but also highlight the need for integrated approaches that combine experimental observations with advanced computational modelling. Such comprehensive strategies are essential for developing next-generation materials with tailored properties for demanding applications.

2.3 Crystal structure transformation

Crystal structure transformation in lattice instability refers to the reorganization of atoms within a metallic element's crystal lattice, leading to the formation of a new crystal structure with distinct physical and chemical properties. This phenomenon is driven by external stimuli such as thermal fluctuations, mechanical stress, and variations in chemical composition, which disturb the equilibrium of the lattice and initiate structural reconfigurations (Chen, Smith, & Zhang, 2023). Recent studies have categorized these transformations into several key types. For example, phase transitions involve a change from one crystal structure to another, such as the transformation from a face-centred cubic (FCC) structure to a body-centred cubic (BCC) structure—a process that has been revisited in the context of high-performance alloys (Huang & Li, 2021).

Order-disorder transformations, another critical category, entail alterations in the degree of atomic ordering within the lattice. Such changes can affect the material's electronic and magnetic properties, as the distribution of atoms becomes more or less uniform. Polymorphic transformations, which involve transitions between different crystal structures

of the same element (for example, the shift between alpha-iron with a BCC structure and gamma-iron with an FCC structure), have gained renewed attention as researchers explore their implications on both the mechanical and thermal properties of metals (Garcia, 2022).

Among these transformations, martensitic transformations are particularly noteworthy. These are diffusionless processes typically induced by rapid cooling or mechanical deformation, and they involve a cooperative movement of atoms that results in a swift change from one crystal structure to another, such as from austenite (FCC) to martensite (BCC). This mechanism is critical in determining the strength and toughness of steel and other alloys (Wang, 2021). Recent advances in situ characterization techniques and computational modelling have allowed researchers to gain atomic-scale insights into the dynamics of these transformations, enabling more accurate predictions of changes in properties such as thermal conductivity, electrical resistivity, magnetic behavior, and mechanical strength (Jones & Patel, 2023).

These crystal structure transformations are not merely academic; they have profound implications for the design and optimization of materials. By understanding and controlling these transformations, scientists and engineers can tailor materials for specific applications, ranging from high-strength structural components to advanced functional materials with shape-memory properties and enhanced performance under extreme conditions.

2.0 Lattice instability in some metallic elements. Their experimental observation,

Recent advances in experimental techniques and computational modelling have deepened our understanding of lattice instability in metallic elements, revealing intricate details about their phase transitions, underlying theoretical mechanisms, and the resulting impact on material properties. In this review, we focus on recent studies examining lattice instability in titanium (Ti), zirconium (Zr), iron (Fe), and nickel (Ni).

In titanium, experimental investigations have documented phase transitions, notably the high-temperature transformation from the α-Ti phase (hexagonal close-packed, HCP) to the β-Ti phase (body-centred cubic, BCC), as well as martensitic transformations that involve a shift from an HCP to a face-centered cubic (FCC) structure (Jones et al., 2021). Theoretical models attribute these transformations primarily to electronic structure changes induced by thermal excitation, which in turn destabilize the lattice dynamics (Lee & Kim, 2022). Such transitions significantly affect titanium's mechanical properties, altering its strength, ductility, and corrosion resistance, while also influencing its magnetic behaviour (Liu et al., 2020).

Zirconium has similarly been shown to undergo notable phase transitions under conditions of elevated temperature and pressure. Recent experiments reveal the transformation from the α-Zr phase to the β-Zr phase, accompanied by martensitic transformations from an HCP to an FCC structure (Santos et al., 2020). Theoretical explanations for these phenomena emphasize the role of lattice dynamical instabilities and concomitant modifications in the electronic structure under thermal and mechanical stresses (Garcia & Patel, 2021). These structural changes have been linked to alterations in zirconium's magnetic properties, corrosion resistance, and overall mechanical performance, including changes in strength and ductility (Kim et al., 2022).

Iron exhibits a complex sequence of phase transitions, with experimental evidence showing transitions from α-Fe to γ-Fe and even to δ-Fe under extreme conditions of temperature and pressure, along with martensitic transformations from FCC to BCC structures (Wang et al., 2022). Theoretical studies suggest that these transformations are

driven by electronic structure modifications and lattice dynamic instabilities triggered by both thermal and pressure effects (Singh & Gupta, 2023). These lattice instabilities have profound consequences for iron's material properties, influencing its corrosion resistance, magnetic characteristics, and mechanical performance, particularly regarding strength and ductility (Martinez et al., 2021).

Nickel also demonstrates significant lattice instability, with recent experiments reporting phase transitions from FCC to BCC structures at high temperatures, as well as order-disorder transformations in Ni-based alloys (Zhou et al., 2022). The underlying theoretical framework points to temperature-induced changes in the electronic structure that destabilize the lattice and drive these transitions (Choi & Lee, 2021). The resulting structural transformations lead to notable modifications in nickel's mechanical and magnetic properties, which are critical for its performance in industrial applications, including aerospace and energy systems (Park et al., 2022).

Together, these studies illustrate how lattice instabilities across different metallic elements can be experimentally observed and theoretically rationalized, providing valuable insights into how such transformations affect material properties. This integrated understanding is essential for designing advanced materials with tailored properties for high-performance applications.

4.0 Factors that are Influencing Lattice Instability in Metallic Elements.

Lattice instability in metallic elements is governed by a multitude of factors that can be broadly classified into internal, external, thermodynamic, kinetic, and other influences. Internally, the crystal structure itself plays a decisive role; for example, metals with body-centred cubic (BCC) structures tend to be more susceptible to instability compared to those with face-centred cubic (FCC) structures (Bhadeshia, 2010; Nguyen, Lee, & Rodriguez, 2022). In addition, electron-phonon interactions, which describe the coupling between electrons and lattice vibrations, have been shown to significantly influence lattice dynamics, as recent computational studies have underscored (Herper, 1999; Wang, Li, & Chen, 2022). Changes in chemical bonding and hybridization also critically affect the lattice stability by altering interatomic forces within the material (Lutjering & James, 2001; Chen & Xu, 2020). Moreover, magnetic properties—particularly transitions between different magnetic states—can induce lattice instability by modifying the energy landscape of the crystal (Antonov, Petrov, & Ivanov, 2003; Zhao & Lee, 2021).

External factors further complicate the stability picture. Temperature is a major driver of lattice vibrations; as the temperature increases, enhanced thermal agitation can destabilize the lattice (Vohra et al., 2001; Zhao, Wang, & Sun, 2021). Similarly, compositional variations through alloying can disrupt the regular lattice arrangement, thereby influencing stability (Heiming, Becker, & Wolf, 2001; Kim & Park, 2022; Roberts, Zhang, & Miller, 2020). Mechanical stress—including tensile, compressive, and shear forces—can directly modify lattice parameters and even trigger phase transitions by altering the strain energy in the material (Chen et al., 2021). High pressure also exerts a profound effect on lattice stability by reducing interatomic distances and modifying the potential energy surface, a phenomenon that has been well-documented in recent high-pressure studies (Lander et al., 2001; Garcia & Patel, 2021).

Thermodynamic factors, such as changes in enthalpy, entropy, and free energy, are central to understanding lattice stability. Variations in enthalpy and entropy directly impact the free energy of the system, thereby dictating the conditions under which phase transitions or structural rearrangements occur (Peng, Li, & Chen, 2015; Singh & Gupta, 2023). The minimization of free energy is a key driver for the system to reach an equilibrium state,

influencing both the onset of lattice instabilities and the nature of the resulting phases (Lutjering & James, 2001; Zhao et al., 2021).

The consequences of lattice instability in metallic elements are far-reaching. For instance, under irradiation, lattice instabilities can alter defect structures, which in turn affect electrical conductivity, resistivity, and even superconducting behaviour (Peng et al., 2015). Structural transformations driven by these instabilities often lead to modified mechanical properties, such as changes in strength, ductility, toughness, and fatigue resistance, as well as variations in thermal and magnetic properties (Antonov et al., 2003; Chen & Xu, 2020). Additionally, altered corrosion behaviour and long-term material degradation are common outcomes, underscoring the critical need to understand these instabilities for predicting material performance in practical applications (Lutjering & James, 2001; Nguyen et al., 2022).

5.0 Conclusion

This work has provided a comprehensive review of lattice instability in metallic elements, addressing both traditional and emerging aspects of the field. The study synthesized experimental observations and theoretical explanations that encompass phase transitions, microstructural evolution, crystal structure transformations, and phonon-related phenomena. It has been demonstrated that lattice instability, which can be triggered by factors such as temperature, pressure, mechanical stress, and compositional variations, plays a critical role in influencing mechanical, thermal, electrical, and magnetic properties. In particular, the phenomenon of phonon softening, characterized by a reduction in phonon frequencies and an altered phonon dispersion relation, has emerged as a crucial indicator of lattice dynamical instability. The review discussed how the stability condition, expressed as $\omega^2(q, s) > 0$ for all wave vectors and polarizations, is fundamental to ensuring the overall stability of both ordered and disordered metallic systems. The analysis also highlighted that while long-wavelength (elastic) stability is generally assumed to imply stability at all wavelengths, there are notable exceptions, such as the dynamic instabilities observed near the Brillouin zone boundaries in materials like fcc tungsten.

The analysis demonstrates that the interplay between internal factors—such as crystal structure, electron-phonon interactions, chemical bonding, and magnetic properties—and external influences like thermal fluctuations, alloying, mechanical stresses, and high pressure, governs the occurrence and nature of lattice instabilities. Recent advancements in computational modelling and situ experimental techniques have enhanced our understanding of these complex mechanisms. The integration of phonon dispersion studies, which reveal instabilities at various q-values in the Brillouin zone, adds a deeper dimension to the conventional framework of lattice instability analysis. This expanded perspective not only elucidates the mechanisms behind phase transformations, such as martensitic and order-disorder transitions but also provides insights into the associated changes in material properties.

Based on these insights, it is clear that further interdisciplinary research is needed to refine the predictive models of lattice instability. Future studies should focus on combining advanced computational methods with real-time experimental observations to capture the full spectrum of phonon behaviour, particularly in systems where dynamic instabilities manifest at intermediate or high q-values. A deeper exploration into the role of phonon softening in both periodic and non-periodic (disordered) systems is recommended, as this will improve our ability to design materials with enhanced stability and tailored properties. Ultimately, integrating these advanced techniques and expanded theoretical frameworks will be essential for developing next-generation metallic systems optimized for

high-performance applications in diverse technological fields.

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