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SPINTRONIC POTENTIAL OF THE BeFeCd SEMI-HEUSLER ALLOY: AN AB INITIO INVESTIGATION

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ABSTRACT

This study comprehensively investigated the structural, elastic, electronic, magnetic and thermodynamic characteristics of the BeFeCd semi-Heusler alloy via density functional theory with the generalized gradient approximation. The alloy crystallizes in the F$\overline{4}$3m space group, with Be, Cd and Fe atoms occupying the (0, 0, 0), (1/4, 1/4, 1/4) and (3/4, 3/4, 3/4) Wyckoff positions, respectively. Structural optimization yielded an equilibrium lattice parameter of 5.487 Å for the mechanically stable configuration. The calculated elastic constants (C_{11} = 195.48 GPa, C_{12} = 105.07 GPa, C_{44} = 16.44 GPa) satisfy the Born stability conditions, confirming the robustness of the crystal structure. The calculated Poisson's ratio (0.412), bulk modulus (135.21 GPa), shear modulus (24.99 GPa) and B/G ratio (5.41) suggest that the alloy combines metallic bonding characteristics with ductile mechanical behavior and has relatively low compressibility. Electronic band structure and density of states analyses revealed that the alloy possesses metallic conductivity dominated by Fe-3d electronic states. Magnetic calculations indicate a total magnetic moment of 2.2 μB per formula unit, suggesting ferromagnetic ordering. The thermodynamic properties evaluated through the Debye model, including vibrational energy, free energy, entropy and heat capacity, exhibit temperature-dependent trends that are consistent with those of typical semi-Heusler alloys. The Debye temperature was determined to be 266.242 K. Overall, these results suggest that BeFeCd is a mechanically stable, metallic and magnetically active semi-Heusler alloy with promising potential applications in spintronics and magnetoelectronics.

1. INTRODUCTION

Half-Heusler (HH) compounds with the general formula XYZ have attracted sustained attention due to their structural adaptability and multifunctional electronic properties [1–3]. The crystallization of these intermetallic systems occurs predominantly in the cubic F$\overline{4}$3m structure, enabling systematic tuning of electronic dispersion and magnetic ordering through compositional variation. The interplay between covalent p–d hybridization and metallic bonding leads to a wide spectrum of electronic behaviors, including semiconducting, semimetallic, and half-metallic characteristics [4,5]. Beyond the scope of conventional magnetic applications, half-Heusler alloys have emerged as a pivotal element in the realm of spin-dependent transport research. The exchange splitting of transition-metal d states has been shown to generate highly asymmetric spin channels in the vicinity of the Fermi level, thereby enabling substantial spin polarization [6,7]. These properties are critical for the functionality of spin injection, magnetic tunneling, and spin filtering devices. Furthermore, several Heusler systems have been predicted and experimentally verified to exhibit half-metallicity or topologically non-trivial band structures, thereby reinforcing their relevance for advanced magneto-electronic technologies [8–10]. A particularly compelling subclass within this family is formed by Fe-based half-Heusler compounds. The partially filled 3D shell of Fe frequently results in the induction of pronounced magnetic moments and robust exchange interactions. These interactions may consequently lead to the manifestation of strong spin asymmetry in the electronic density of states [11,12]. A substantial body of research has demonstrated that theoretical calculations and experimental studies on Fe-containing HH systems, such

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as FeNbSb and FeVSb, have yielded results that indicate structural stability combined with promising magnetic and transport behavior [13,14]. The experimental synthesis techniques of arc melting and spark plasma sintering have been demonstrated to be effective methods for stabilizing Fe-centered half-Heusler phases in their bulk form, as evidenced in the literature [14]. The assessment of material viability is contingent upon a comprehensive consideration of both lattice dynamics and thermodynamic stability. The Debye temperature, phonon dispersion analysis, and quasiharmonic approximations are widely used to assess mechanical robustness and thermal response in newly proposed Heusler materials [15–17]. These investigations offer predictive insight into phase stability prior to experimental realization. Despite the extensive research conducted on Fe-based half-Heusler systems, there are certain compositional combinations that have yet to be explored. Specifically, the Be–Fe–Cd configuration has not been the subject of systematic investigation within the semi-Heusler framework. It is important to consider the strong bonding tendency of Be and the more diffuse p orbitals of Cd when assessing the interaction of these elements with Fe 3d states. This interaction may introduce distinctive hybridization effects, influencing both magnetic exchange and electronic structure. To the best of our knowledge, a comprehensive first-principles analysis of BeFeCd has not yet been reported. The present study aims to provide a systematic ab initio evaluation of the structural stability, elastic behavior, electronic structure, magnetic ordering, and thermodynamic properties of the BeFeCd semi-Heusler alloy. The study will place particular emphasis on the alloy's potential suitability for spin-dependent electronic and magneto-electronic applications. Specifically, the calculated magnetic moment and spin-resolved electronic structure obtained in this study enable a direct assessment of its potential half-metallic tendency, which is essential for spin-dependent transport applications.

2. MATERIALS AND METHOD

A thorough investigation of the BeFeCd semi-Heusler alloy was conducted within the framework of density functional theory (DFT) using the Quantum ESPRESSO package [18]. The electron-ion interaction was described by projector augmented-wave (PAW) pseudopotentials, while the exchange-correlation energy was treated using the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) formulation [19]. The PBE functional was selected due to its proven reliability in predicting equilibrium lattice parameters, magnetic moments, and energetic stability in transition-metal-based Heusler systems. The semi-Heusler crystal structure, classified under the cubic $F\bar{4}3m$ space group, was constructed utilizing the Wyckoff positions Be (0, 0, 0), Cd (1/4, 1/4, 1/4), and Fe (3/4, 3/4, 3/4). A total-energy comparison of several atomic configurations was conducted to identify the energetically most favorable arrangement. The structural optimization was executed employing the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm until the residual atomic forces were diminished to below 0.01 eV/Å and the total energy variations diminished to below 10^{-6} eV. The plane-wave kinetic energy cutoff was systematically tested in the range of 500–600 eV to ensure convergence of total energy and stress tensors. The selected cutoff value corresponds to a regime where total energy variations were less than 1 meV per atom. Convergence analysis is imperative for deriving reliable elastic and magnetic properties in intermetallic systems [20]. The Brillouin zone sampling was performed using the Monkhorst–Pack scheme [21]. To this end, a series of k-point meshes (8×8×8, 10×10×10, and 12×12×12) were examined to assess the convergence of total energy and magnetic moment. The 8×8×8 grid was determined to be adequate, as subsequent refinement yielded negligible energy differences (< 1 meV). Accurate k-point sampling is of particular importance for the description of states near the Fermi level in metallic and near half-metallic systems. Spin-polarized calculations were employed throughout this study due to the presence of Fe atoms with partially filled 3d orbitals, which have been shown to induce exchange splitting and magnetic ordering effects [22]. The independent treatment of spin channels facilitated a comprehensive evaluation of spin-resolved band structures and densities of states (DOS). Total DOS (TDOS) and partial DOS (PDOS) analyses were performed to identify orbital contributions, particularly the role of Fe 3d states near the Fermi level. The elastic constants (C_{11}, C_{12}, C_{44}) were determined using the stress–strain method within the linear elastic regime governed by Hooke's law. Subsequent to the implementation of small symmetry-preserving strains, a recalculation of total energies was conducted to obtain stress tensors. The mechanical stability of the cubic phase was evaluated according to the Born stability criteria, which require $C_{44} > 0$, $C_{11} - C_{12} > 0$, and $C_{11} + 2C_{12} > 0$ [23]. The bulk modulus (B), shear modulus (G), Young's modulus (E),

Poisson's ratio (ν), and the Pugh ratio (B/G) were derived from the calculated elastic constants. These derivatives were obtained using standard Voigt–Reuss–Hill approximations. Thermodynamic properties were evaluated using the Thermo_pw package [24], which is based on density-functional perturbation theory (DFPT). The quasi-harmonic Debye model implemented within Thermo_pw was employed to estimate Debye temperature (θ_D), vibrational free energy, entropy, and heat capacity at constant volume (C_v) as functions of temperature. The calculations were executed within the temperature range of 0–800 K, and the approach toward the Dulong–Petit limit at elevated temperatures was analyzed. This methodology provides insight into the vibrational stability and temperature-dependent behavior of Heusler-type intermetallic compounds.

3. RESULTS AND DISCUSSION

3.1. Structural Properties

The structural and elastic characteristics of the BeFeCd semi-Heusler alloy are fundamental parameters that determine the material's stability and potential functional applications. In this study, the atomic arrangement and crystal symmetry of the alloy were initially evaluated, followed by a thorough examination of the elastic constants and associated moduli that determine its mechanical stability. The initial structure of the alloy was modeled in the $F\overline{4}3m$ space group to match the characteristic $C1_b$ crystal lattice of Heusler compounds. Within this structure, the Be atom occupies the Wyckoff position at the (0,0,0) point, the Cd atom occupies the 4c position at the (1/4,1/4,1/4) location, and the Fe atom occupies the 4b site corresponding to the (3/4,3/4,3/4) coordinate. The representative lattice structure of the BeFeCd semi-Heusler alloy is illustrated in Figure 1.

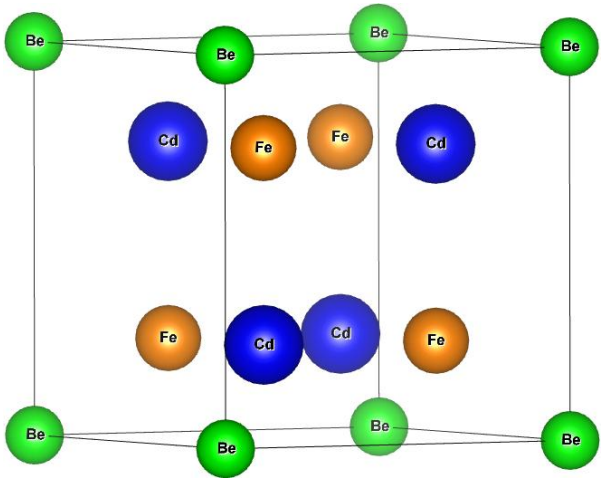


Figure 1. The following is a representation of the unit cell structure of the BeFeCd semi-Heusler alloy. The alloy belongs to the $F\overline{4}3m$ space group and has a $C1_b$ crystal structure.

This configuration corresponds to the standard XYZ stoichiometry of semi-Heusler alloys and exemplifies a regular cubic structure, wherein the positions of atoms within the crystal are constrained by specific symmetry elements [25]. The lattice constant that was obtained as a result of structural optimization was 5.487 Å, which is consistent with the volumetric trends of traditional semi-Heusler compounds. The rearrangement of the atomic bond distances and cell volume during optimization to reach the energy minimum indicates that the system converges to a single stable configuration. Subsequent to structural optimization, the elastic constants were calculated to determine the mechanical stability of the material. Cubic crystals are characterized by three independent elastic constants (C_{11}, C_{12}, and C_{44}), which directly influence both the bond rigidity within the unit cell and the macroscopic mechanical behavior of the material. The elastic constants obtained from the calculations are presented in Table 1.

Table 1. Elastic constants of the BeFeCd semi-Heusler alloy (C_{11}, C_{12}, and C_{44}; GPa)

Material	C_{11}	C_{12}	C_{44}
BeFeCd	195.48	105.07	16.44

The calculated elastic constants for BeFeCd are C_{11} = 195.48 GPa, C_{12} = 105.07 GPa, and C_{44} = 16.44 GPa. These values explicitly satisfy the Born stability criteria ($C_{11} > 0$; $C_{44} > 0$; $C_{11} - C_{12} > 0$; $C_{11} + 2C_{12} > 0$). Consequently, the alloy has been shown to generate a mechanically stable phase [26]. In order to further validate the reliability of the calculated elastic parameters, it is useful to compare their magnitude with those of representative Heusler and half-Heusler systems reported in the literature. Due to the absence of experimental elastic data for BeFeCd, a direct comparison is not currently feasible. However, the obtained single-crystal elastic constants (C_{11}, C_{12}, C_{44}) and the derived polycrystalline moduli (*B*, *G*, and *E*) fall within the range typically reported for Fe-based cubic half-Heusler compounds. For instance, experimental studies of half-Heusler systems, such as NiTiSn, have been extensively utilized as benchmarks for validating first-principles predictions of elastic stiffness [27]. Moreover, theoretical reports have indicated the existence of a chemically related Heusler-type compound, Be_2FeCd, which possesses comparable order of magnitude elastic constants and bulk/shear moduli, thereby substantiating the internal consistency of the present results [28]. The polycrystalline moduli were obtained using the Voigt–Reuss–Hill (VRH) averaging scheme, which is commonly adopted to enable comparison between single-crystal calculations and experimentally measured polycrystalline data [29]. The bulk modulus (*B* = 135.21 GPa), derived from the elastic constants, indicates that the alloy has low compressibility and tends to maintain its volumetric stability under external pressure. Conversely, the shear modulus (*G*) is determined to be 24.99 GPa, suggesting that the Fe–Cd and Fe–Be bonds demonstrate enhanced flexibility in response to shear forces. This behavior is attributed to the metallic nature of these bonds, which is in line with the established principles of metallurgy. The Young's modulus, defined as *E* = 70.58 GPa, offers insights into the material's stiffness within the linear elastic region. The Pugh ratio (*B/G* = 5.41) clearly indicates that the alloy exhibits ductile behavior. This value is significantly greater than the 1.75 threshold and is consistent with the typical behavior observed in materials characterized by a predominant metallic bonding nature [30]. The Poisson's ratio, defined as *v*, was calculated to be 0.412, a value that further substantiates the prevalence of metallic bonding characteristics. Furthermore, the anisotropy factor of a material, defined as the ratio of the material's principal axes to its unit cell, is measured at 0.37. This value deviates from 1, indicating that the alloy's mechanical properties are contingent on the crystal orientation, thereby exhibiting elastic anisotropy.

A comprehensive analysis of the structural and elastic parameters indicates that the BeFeCd semi-Heusler alloy is a stable material with low compressibility, a distinctly metallic character, and ductile behavior. These properties render the alloy suitable for demanding applications in the electronic, magnetic, and mechanical domains. Its mechanical stability and metallic bond characteristics are similar to those of semi-Heusler compounds, which have gained prominence in spintronic and thermoelectric research in recent years [31]. To further assess geometrical compatibility within the cubic lattice, the relative atomic size differences among Be, Fe, and Cd were quantitatively evaluated. Atomic size disparity is known to influence lattice strain and phase stability in intermetallic compounds, particularly when elements occupy well-defined crystallographic sites. The metallic radii used in this analysis are: Be = 112 pm, Fe = 126 pm, and Cd = 148 pm [32]. The relative size deviation (δ) between atomic pairs was calculated using: $\delta = (|r_i - r_j| / r_j) \times 100$. Where r_i and r_j represent the metallic radii of the corresponding elements. The calculated mismatch values are:

Be–Fe:11.11%
Fe–Cd:14.86%
Be–Cd: 24.32%

The Be–Fe and Fe–Cd differences remain below the commonly referenced 15% empirical threshold, suggesting that these pairs are geometrically compatible within the semi-Heusler framework. Although the Be–Cd mismatch exceeds this value, semi-Heusler compounds are ordered intermetallic systems in which atomic positions are symmetry-constrained rather than randomly substituted. In such systems, electronic structure effects particularly transition-metal d-state hybridization can compensate for moderate size disparities. In the present case, the Fe-centered bonding environment and the dominant Fe-3d contribution near the Fermi level indicate that electronic stabilization likely plays a decisive role in maintaining cubic phase integrity. Therefore, despite the relatively large Be–Cd radius difference, the combined elastic stability and electronic structure results support the structural viability of the BeFeCd semi-Heusler phase.

3.2. Electronic Properties

The electronic structure of the BeFeCd semi-Heusler alloy is a critical factor in determining the metallic character, magnetic behavior, and performance of the alloy in potential spintronic applications. Consequently, a thorough examination of the band structure, total density of states (TDOS), and projective density of states (PDOS) has been conducted. It is evident from the calculations of the electronic band structure in the high-symmetry direction that the valence and conduction bands intersect the Fermi level in both the spin-up and spin-down channels. This intersection validates the hypothesis that the semi-Heusler alloy does not exhibit an energy gap for electronic carriers, thereby demonstrating distinct metallic conductivity [33]. The metallic character of BeFeCd can also be rationalized within the framework of the 18-valence-electron rule commonly applied to semi-Heusler compounds. According to this empirical principle, systems containing 18 valence electrons per formula unit tend to exhibit semiconducting ground states due to the complete filling of bonding states below the Fermi level [34]. This behavior has been widely discussed in Heusler systems in connection with electron counting schemes and band filling arguments [35]. In contrast, BeFeCd possesses a total of 12 valence electrons (Be: 2, Fe: 8, Cd: 2), which is significantly lower than the 18-electron requirement. As a result, the bonding states are not fully occupied, and partially filled bands are expected to cross the Fermi level. Therefore, the absence of an energy gap and the finite density of states at the Fermi level (EF) are fully consistent with its non-18-electron configuration. The calculated electronic band structure and corresponding density of states are presented in Figures 2 and 3, respectively.

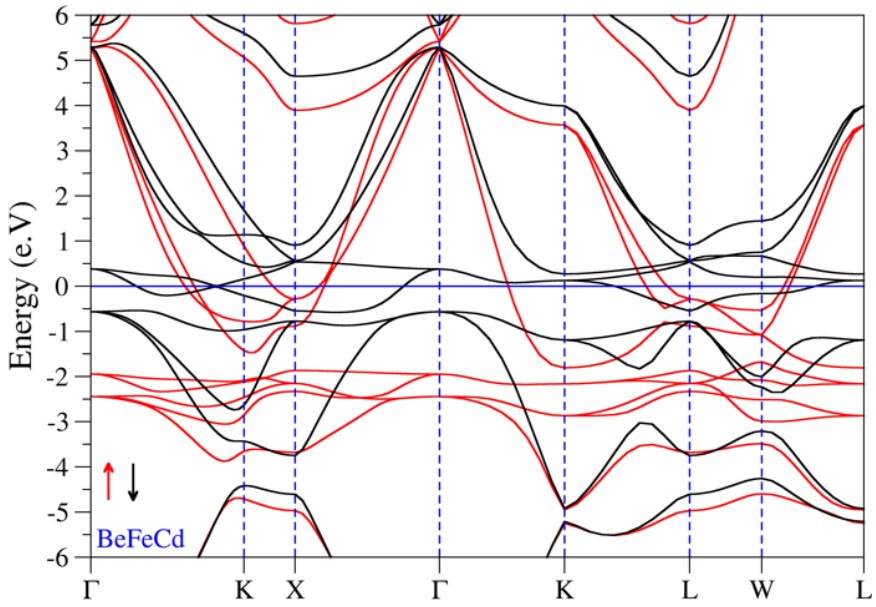


Figure 2. Electronic band diagram of the BeFeCd semi-Heusler alloy.

Density of states (DOS) analyses provide a more detailed perspective on the origin of metallic behavior. The DOS results unequivocally demonstrate the dominant role of the 3d orbitals of the Fe atoms around the Fermi level. This band contribution is consistent with the high spin polarization tendencies reported in the literature for Fe-based semi-Heusler alloys [36]. The s and p orbitals of the Be and Cd atoms generate a limited density in the lower regions of the band structure. Concurrently, the width and energy position of the Fe-3d bands, which constitute the primary component of conductivity, substantiate the robust metallic character of the alloy. Spin-polarized calculations revealed that the BeFeCd alloy has not only a metallic but also a ferromagnetic structure. The calculation of the total magnetic moment per unit cell as 2.2 μB indicates that the spin splitting of the d-electrons on the Fe atoms leads to magnetic ordering. This magnetic moment value is consistent with the ferromagnetic behavior previously reported in Fe-based semi-Heusler compounds and is thought to originate from the spin asymmetry of d orbital hybridization [37].

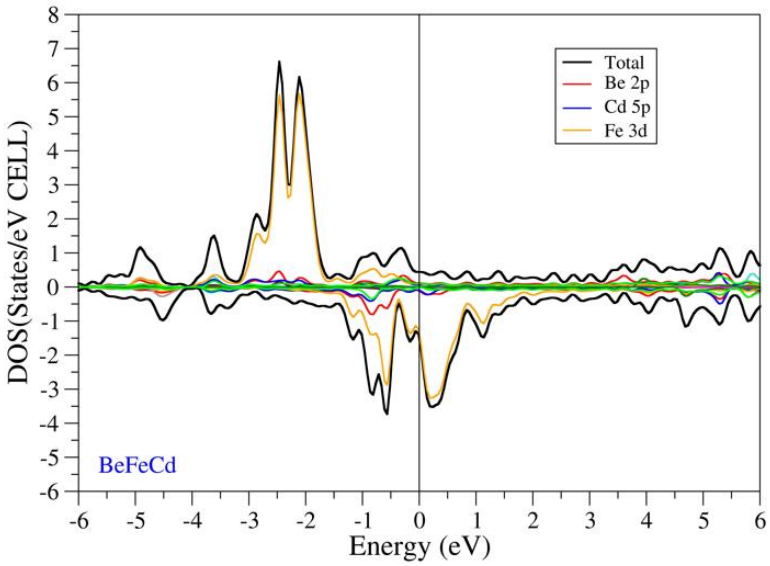


Figure 3. DOS of the BeFeCd semi-Heusler alloy.

When the metallicity, magnetization, and spin separation of the electronic structure are evaluated together, the BeFeCd alloy could be a potential magnetoelectronic and spintronic candidate material. Indeed, recent studies have reported that transition metal-containing semi-Heusler compounds offer structures suitable for use in spin-torque-based devices, spin filters, and spin-valve structures because of their high spin polarization, low energy loss, and band structure compatibility [38]. The Fe-3d dominant band structure and pronounced ferromagnetic tendency of the BeFeCd alloy are consistent with these properties. The obtained electronic band structure, DOS, and magnetic moment results reveal that the BeFeCd semi-Heusler alloy offers advantageous electronic properties such as high conductivity, ferromagnetic character, and strong d-orbital contributions around the Fermi level. These results suggest that the alloy is a suitable candidate for theoretical evaluation of spintronic components and provide an important basis for future experimental studies.

3.3. Thermodynamic Properties

The temperature-dependent thermodynamic behavior of the BeFeCd semi-Heusler alloy is critical for understanding the dynamic stability, heat storage capacity, and atomic vibration characteristics of the alloy at different temperatures. In this context, on the basis of the Debye model, the temperature-dependent changes in the vibration energy, free vibration energy, entropy, and heat capacity of the alloy at a constant volume (C_v) were examined in detail. All calculations were performed in the 0–800 K range, and the relevant curves are presented graphically in Figures 4, 5, 6, and 7.

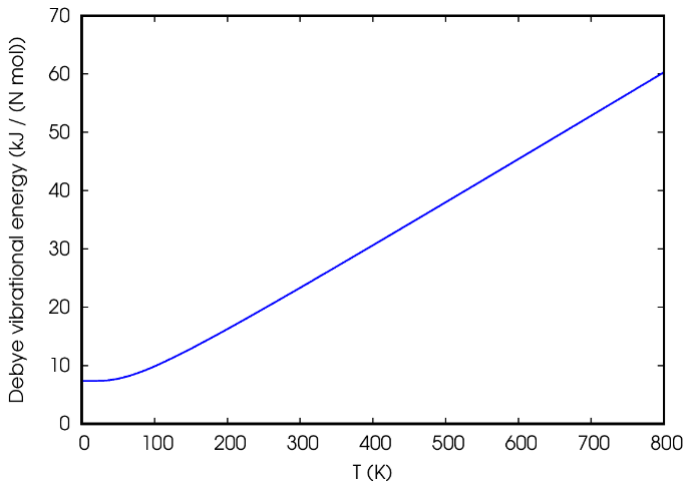


Figure 4. Graph of vibration energy as a function of temperature.

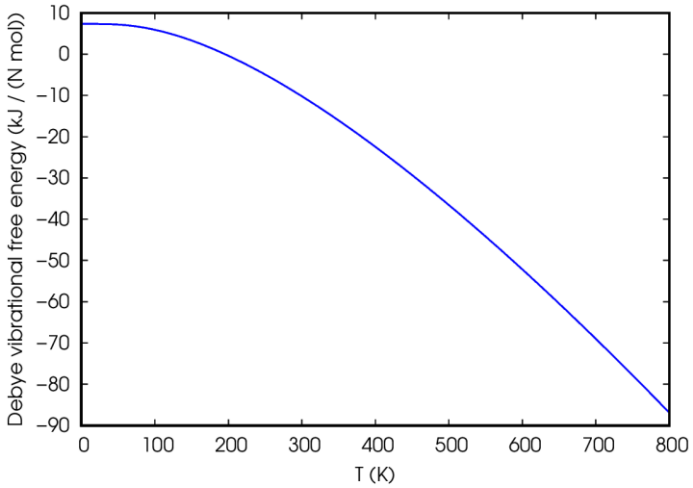


Figure 5. Graph of free vibration energy as a function of temperature.

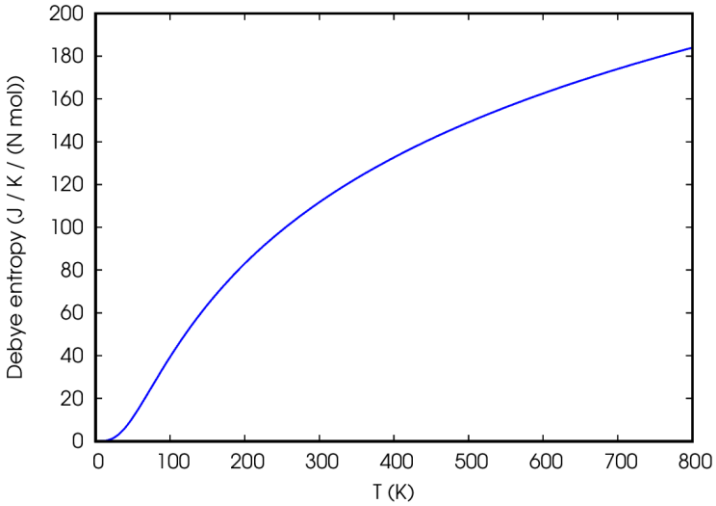


Figure 6. Graph of entropy as a function of temperature.

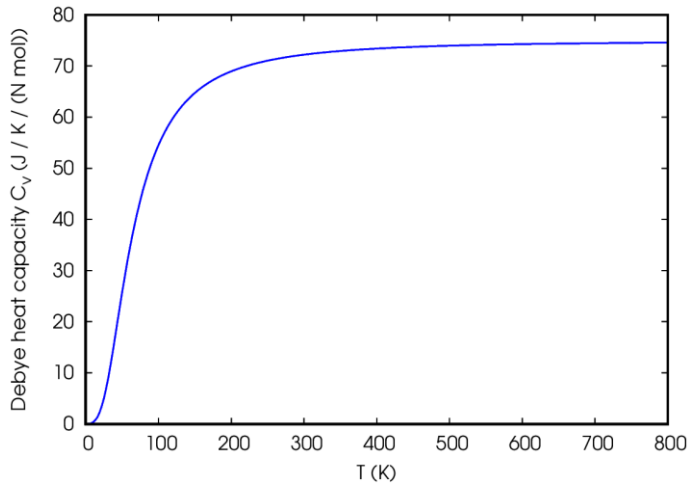


Figure 7. Graph of heat capacity as a function of temperature.

The choice of the 0–800 K temperature interval is motivated by both physical and practical considerations. As illustrated in Figure 7, the heat capacity (C_v) gradually approaches the Dulong–Petit

limit at elevated temperatures, indicating the classical saturation regime of lattice vibrations [39]. Extending the calculations up to 800 K enables a clear observation of this asymptotic behavior. Moreover, although the melting temperature of BeFeCd has not yet been experimentally determined, the selected range remains within a thermodynamically meaningful regime for intermetallic systems. In addition, this interval exceeds typical operating temperatures of spintronic and magnetoelectronic devices (generally below ~400 K), thereby ensuring technological relevance. The Debye model, a cornerstone of thermal analysis, is predicated on the harmonic vibrations of atoms within the crystal lattice, ensuring exceptional precision, particularly at low and medium temperatures. With this model, the Debye temperature was calculated and found to be 266.242 K for the BeFeCd alloy. This value indicates that the alloy has a crystal lattice structure with medium rigidity. An increase in the Debye temperature corresponds to an increase in the energy demands of the material's vibration modes. Consequently, the calculated value indicates that BeFeCd manifests the properties of a medium-hardness material with regard to heat conduction and phonon behavior [40]. Conversely, the vibration energy exhibited a monotonic increasing trend as the temperature increased. This outcome is in full accordance with the fundamental thermodynamic principle that the kinetic energy of atoms within a crystal increases with temperature. The calculated curve is displayed in Figure 4, which shows that the curve increases more slowly at low temperatures and more rapidly at higher temperatures.

This phenomenon can be attributed to the temperature-dependent energy distribution of the phonons. The concept of free energy is derived by evaluating the total energy in conjunction with entropic contributions. An examination of Figure 5 reveals a decreasing profile of the free energy curve as the temperature increases. This phenomenon can be attributed to the increase in system disorder with increasing temperature, as well as the increasingly prominent role of entropy in determining free energy. From a thermodynamic perspective, this phenomenon is a predicted trend for all crystalline materials, and the BeFeCd alloy adheres to this fundamental physical principle [41]. Entropy is defined as a quantitative measure of disorder in a system. A close examination of Figure 6 reveals a continuous and increasing trend in entropy with temperature, albeit not a linear relationship. The curve clearly exhibits a more pronounced upward inclination and an escalation in disorder, particularly in the high-temperature region. This behavior observed for the BeFeCd alloy is consistent with the results reported in the literature regarding the phonon distributions of semi-Heusler compounds.

When examining Figure 7, which shows the temperature-dependent change in heat capacity at a constant volume, C_v increases rapidly at low temperatures. However, as the temperature increases above approximately 100 K, the rate of increase slows down and approaches the Dulong–Petit limit. This limit is expressed by the relationship $C_v \approx 3Nk_B$ and represents the upper limit expected to be reached by crystalline materials at high temperatures. The conventional approach to this limit in the BeFeCd alloy substantiates the hypothesis that the lattice vibrations of the material comport with physical models [42]. It should be emphasized that the thermodynamic trends predicted within the Debye approximation describe vibrational behavior under the quasi-harmonic assumption. However, independent phonon dispersion calculations reveal the presence of imaginary modes, indicating that the ideal cubic phase may not be dynamically stable at 0 K within the harmonic approximation. Therefore, the Debye-based thermodynamic results reflect temperature-dependent vibrational trends rather than definitive proof of complete dynamical stability. The alloy's reliable semi-Heusler profile is evident in the consistent variation in parameters such as vibration energy, free energy, entropy, and heat capacity. This profile indicates the alloy's stability and predictable physical behavior under thermal conditions. These properties render the BeFeCd alloy a potential candidate not only for electronic and magnetic applications but also for device designs where high-temperature thermodynamic performance is critical.

4. CONCLUSION

A comprehensive first-principles investigation of the structural, elastic, electronic, magnetic, and thermodynamic properties of the BeFeCd semi-Heusler alloy has been presented. Structural optimization confirmed that the alloy crystallizes in the $C1_b$ type cubic phase within the $F\overline{4}3m$ space group. The calculated elastic constants satisfy the Born stability criteria, confirming mechanical stability against small elastic deformations. The relatively high bulk modulus indicates low compressibility, while the moderate Young's modulus suggests a balanced elastic response. The Pugh ratio (B/G), defined

as the ratio of bulk modulus to shear modulus, exceeds the critical value of 1.75, indicating ductile mechanical behavior. The calculated Poisson's ratio further supports the predominance of metallic bonding characteristics. The elastic anisotropy factor, defined for cubic crystals as $A = 2C_{44}/(C_{11}-C_{12})$, deviates from unity, indicating orientation-dependent mechanical response typical of semi-Heusler systems. Electronic band structure and density of states analyses reveal metallic conductivity characterized by band crossings at the Fermi level and dominant Fe-3d contributions. The calculated total magnetic moment of 2.2 μB per formula unit confirms a ferromagnetic ground state originating from spin-split Fe-d states. These results collectively indicate that BeFeCd exhibits electronic and magnetic features compatible with potential magnetoelectronic and spintronic applications. Thermodynamic properties evaluated within the Debye approximation show physically consistent temperature-dependent trends for vibrational energy, entropy, and heat capacity. However, separate phonon dispersion calculations reveal the presence of imaginary modes, suggesting that the ideal cubic phase may not be dynamically stable within the harmonic approximation at 0 K. This indicates a possible tendency toward lattice distortion or defect-assisted stabilization. Therefore, while the alloy is mechanically stable, further investigations involving finite-temperature phonon calculations or structural distortions may be necessary to fully clarify its dynamical ground state. Overall, the combined mechanical robustness, metallic conductivity, and ferromagnetic character of BeFeCd suggest that the alloy warrants further theoretical and experimental exploration, particularly in the context of spin-dependent transport and magnetically functional materials.

Statement of Research and Publication Ethics

The study complies with research and publication ethics.

Artificial Intelligence (AI) Contribution Statement

Artificial intelligence (AI) tools (ChatGPT, OpenAI) were used solely for language refinement and minor editorial assistance, and for verifying the consistency of computational interpretations. All scientific analyses, results, figures, and conclusions were generated exclusively by the authors.

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