First-principles investigations of physical properties of Nd doped FeSi compound

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ABSTRACT
The structural, electronic, magnetic and thermodynamics properties of the NdFeSi intermetallic compound are studied using the full potential linearized augmented plane wave plus local orbital method, which is based on the theoretical framework of the density functional theory. We calculated the structural properties, in terms of the lattice constant, bulk modulus, first derivative of bulk modulus, and minimum volume. We calculated the electronic properties by considering the band structure, as well as the total and partial density of states. Electronic properties are confirmation that the NdFeSi intermetallic compound exhibits a metallic nature due to Nd-f state. The magnetic properties correlate with the magnetic moment. We determined that this compound's magnetic moment is 7.02610 μB. We investigated thermal behavior in terms of the Grüneisen parameter γ, the bulk modulus B_0, the Debye temperature θ_D, and the entropy S with different temperatures and pressure ranges. All these results indicate that the NdFeSi compound is used in spintronic applications.
KEYWORDS
DFT • electronic properties • density of state • rare earth element

Introduction

Researchers have been exploring the unique and exciting properties of rare-earth intermetallic compounds, which include a high melting point, good temperature ductility, high strength, hardness, low specific weight, corrosion resistance, various temperature mechanical properties, and the use of electronic and magnetic properties [1]. Compounds such as the RETX eSolid-state physics contains compounds such as the RETX equal-atomic ratio stoichiometry arrangement and approximately 2,000 combinations [2], types of crystal structures in crystallography [3]. Researcher-led exploration exercises and further development in this field are ongoing. This has improved human society. The study of RETX-type materials has explored electronic, magnetic, and thermodynamic behavior, and these materials show different kinds of industrial applications. It has much potential in multiple sectors, such as aviation, automobiles, spintronics, electrical, and

electronics industries [4,5]. Rare-earth intermetallic compounds have a magnetic nature because they contain incompletely filled 4-f electron orbitals. When the temperature rises above room temperature, they show a ferromagnetic core with high spin polarization [5]. Previous publications demonstrated that the magnetic nature of NdFeSi, GdFeSi, TbFeSi, and LaFeSi materials, as well as REFeSi (RE=Nd, Gd, and Tb), exhibits a ferromagnetic nature at Curie temperature T_c = 25 K for NdFeSi, 135 K for GdFeSi, and 125 K for TbFeSi, while LaFeSi exhibits a paramagnet nature [6]. All elements of the lanthanide's series have paired and unpaired electrons in their inner 4-f orbits. There are 4-f uncompleted subshells in the electronic configuration of Nd ([Xe] $4f^4$ $6s^2$) due to the uncompleted 4-f electron orbitals. RETX rare-earth intermetallic compounds show a magnetic nature due to the uncompleted 4-f electron orbital's

In this research paper, we have examined the electronic, magnetic, and thermal behaviours of the NdFeSi compound using the density functional theory (DFT), which relies on fundamental concepts such as the Kohn-Sham (KS) equation and the self-consistent field (SCF) [7,8]. We conducted structural, electronic, and magnetic calculations using the WIEN-2K software [9], and we also utilized this software to investigate the thermal behaviour. However, this was only feasible when we interfaced WIEN-2K with GIBBS2 software. GIBSS2 software is based on the Debye model [10]. The NdFeSi compound has a CeFeSi-type tetragonal crystal structure, and the space group is p4/nmm [11,12]. We looked at the crystal structure, energy E - volume V curves, bulk modulus B_0, and a derivative of bulk modulus B_0'. We studied the electronic behaviour using band diagrams and the total and partial density of state (TDOS and PDOS, respectively). We also looked at the thermal behaviour using the Gruneisen parameter γ, the bulk modulus B_0, the Debye temperature (θ_D), and the entropy (S). We studied this over a wide range of temperatures and pressures.

Method of calculations

In this paper, a computational approach was used. We studied the NdFeSi material's electronic, magnetic, and thermodynamic properties using the FPLAPW+LO method and the general gradient approximation (GGA) based on DFT [13–15]. We used the Birch-Murnaghan equation (EOS) to find the structural properties of the NdFeSi material [16]. We selected a cutoff energy of 6.0 Ry and three k-mess points under the high-symmetry Brillouin zone for the SCF calculation. ne. In this process, we choose a charge of approximately 0.0001 ec for crystal convergence. The muffin tin sphere radius (RMT) is the small atomic electron cloud sphere radius in a unit cell. RMT plays an important role in the calculation of physical properties. If we need more plane waves, then we require a large RMT. Many plane waves contribute significantly to the calculation's accuracy. However, if we heavily rely on RMT, the surface charge will leak. Given that no center charge should be present, its value must be minimal. Its value should be meager, as there is no core charge leaking from its surface. If the charge leaks, the RMT's value fluctuates, either increasing or decreasing. This on the core surface, there is no charge leakage. We keep the RMT value low to allow for the retention of more plane waves. In our calculation, we have taken RMT 2.50 a.u. for Nd and 2.00 a.u. for Fe and Si. For our SCF calculations, we have chosen lattice parameters a_0 = b_0 = 4.031 Å and c_0 = 6.828 Å for NdFeSi (CeFeSi type tetragonal

crystal structure) shown in Table 1. We found the Fermi energies to be 0.64630 electron volts (Table 2). We investigated the magnetic properties of the material using GGA and DFT. We used GIBBS2 software for the material's thermal behaviour. It's based on the Debye model.

Table 1. Crystallography data of NdFeSi compound such as space group, lattice parameter and atomic position

Compound	Space group	Lattice parameter, Å	Nd	Fe	Si
NdFeSi	p4/nmm (129)	$a_0=b_0=4.031$ $c_0=6.828$	(0.25, 0.25, 0.67)	(0.75, 0.25, 0)	(0.25, 0.25, 0.20)

Table 2. Lattice parameters (a_0, c_0), bulk modulus B_0, the derivative of bulk modulus B_0', minimum energy E_{min}, the volume of unit cell V_0, and the Fermi energy E_F at 0 K for NdFeSi compound

S.N.	Parameter	Symbols	Value	Experimental data
1	Lattice parameters, Å	$a_0=b_0$	4.069	4.031 [18]
		c_0	6.918	6.828 [18]
2	The bulk modulus of material, GPa	B_0	103.7584	
3	derivative of bulk modulus of material, GPa	B_0'	4.3393	
4	The energy at equilibrium condition, Ryd	E_{min}	-44771.811751	
5	Unit cell volume at equilibrium condition, a.u.^{3}	V_0	749.9931	
6	Fermi energy, eV	E_F	0.64630	

Results and Discussion

Structural properties

VESTA software was used to generate the unit cell structure (Fig. 1) of the NdFeSi material [17]. The NdFeSi compound shows a CeFeSi-type tetragonal crystal structure. Birch-Murnaghan equations (EOS) have helped determine structural properties in terms of *E-V* curve, B_0, and B_0'. Table 2 displays the determined values of the structural parameter for the NdFeSi compound. The determined estimations of the lattice constant show remarkable concurrence with experimental values [18–26]. B_0 is an essential parameter
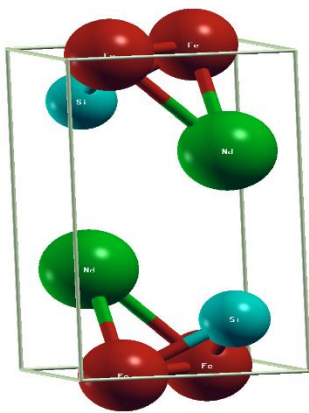

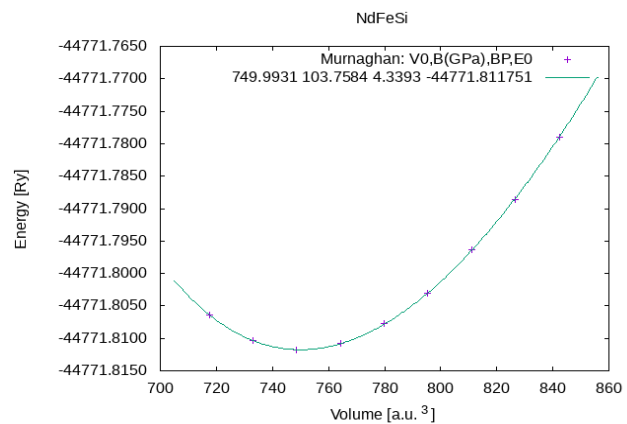**Fig. 1.** Unit cell crystal structure of NdFeSi compound used VESTA software

Fig. 2. Variation of total energy with unit cell volume of NdFeSi compound

of materials in material science and a measure of the material's resistance to compression. The degree of resistance value also increases when B_0 is increased, as shown in Table 2. The literature does not contain any experimental B_0 values. As a result, our measured results are considered predicted; we can use them in future research work. The material's *E-V* curve, as depicted in Fig. 2, provides information about the structural stability curves. Such curves offer NdFeSi compound stability.

Electronic and magnetic properties

Now we are discussing the electronic properties of the NdFeSi compound in terms of band structure, TDOS, and PDOS. We have determined the electronic band diagrams of the NdFesi compound along with spin up and spin down the channel in high symmetry Brillouin zone direction using GGA approximation. In the electronic band diagrams, Fig. 3(a,b) for the NdFeSi compound displays the Fermi level at the origin. In-band graphs, most of the bands lie from -9.5 to 0 eV for the spin-up channel below the Fermi level shown in Fig. 3(a). Similarly, most of the bands lie from -9.0 to 0 eV for the spin-down channel below the Fermi level shown in Fig. 3(b). From Fig. 3(a,b) in the band diagram, we see that the valance and conduction bands overlap among themselves. Therefore, the NdFeSi compound exhibits a metallic character. This result primarily accounts for the unfailing of the Nd-4f ([Xe] 4f46s2) electronic shell. The result is clear, our combination has a metallic nature. We are discussing TDOS and PDOS of the NdFeSi compound shown in Fig. 4. In Fig. 4(a), we can see there are three sharp peaks in the valence and conduction bands.
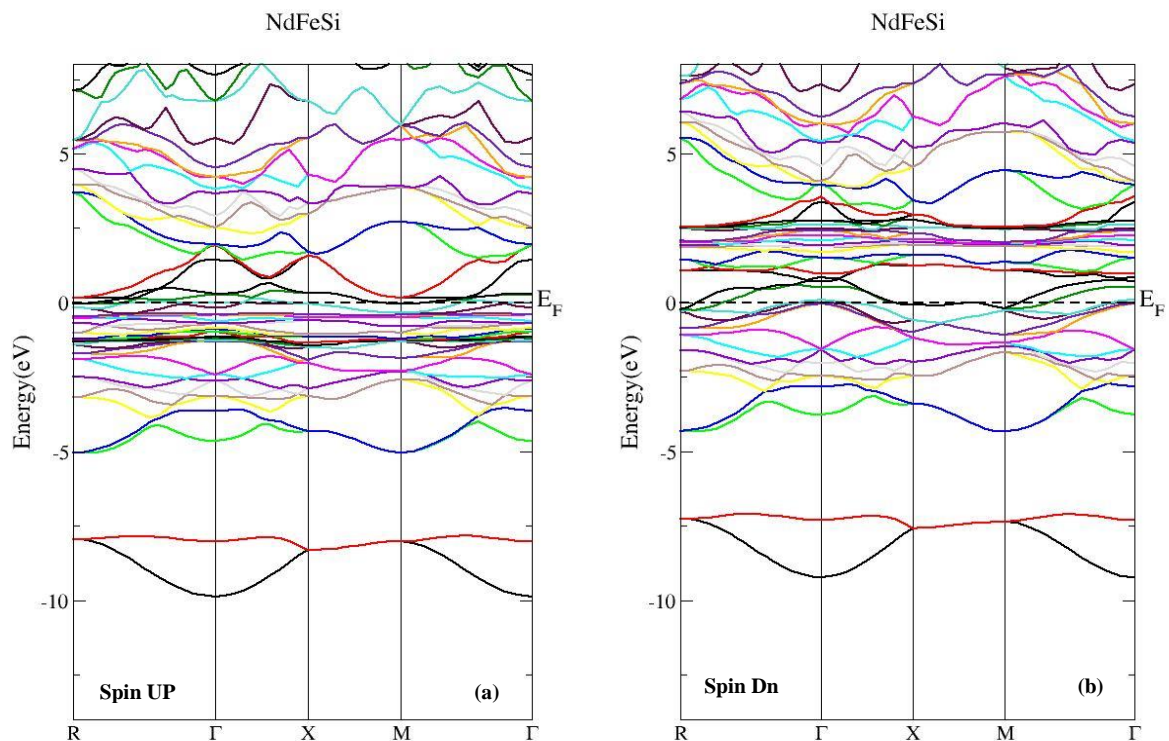

Fig. 3. Electronic band structures of (a) NdFeSi for spin up and (b) NdFeSi for spin down (Dn) using GGA approach
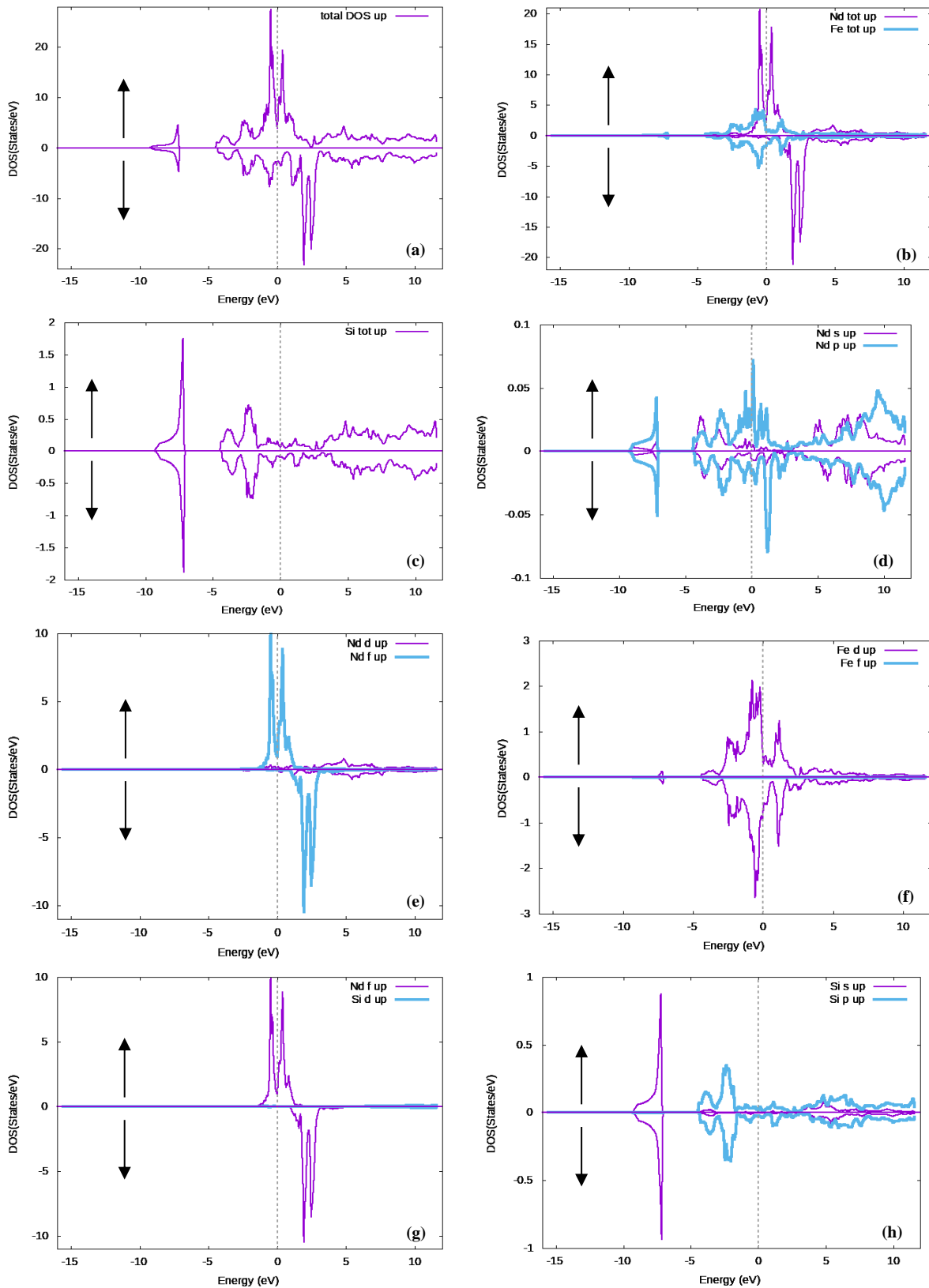
Fig. 4. Density of states(DOS) along with spin up and spin down of (a) NdFeSi-total DOS,
(b) Nd-total DOS and Fe- total DOS, (c) Si-total DOS, (d) Nd-s partial DOS, and Nd-p partial DOS,
(e) Nd-d partial DOS and Nd-f partial DOS, (f) Fe-d partial DOS and Fe-f partial DOS,
(g) Nd-f partial DOS and Si-d partial DOS, (h) Si-s partial DOS and Si-p partial DOS

The first peaks in the valance band correspond approximately to -7.1 eV for the spin-down channel below the Fermi levels, and another two peaks correspond approximately to -7.1 and -0.62 eV for the spin-up channel below the Fermi level. Similarly, in the conduction band, the first peaks approximately belong to 0.63 eV for the spin-up channel above the Fermi level, and another two peaks approximately belong to 1.87 and 2.5 eV for the spin-down channel above the Fermi level.

The sharp peak between -0.62 and 0.63 eV is responsible for the Nd-f electronic shell (Fig. 4(e)), with a minor role for the Fe-d electronic shell (Fig. 4(f)). The sharp peak of -7.1 eV is responsible for the Si-S electronic shell (Fig. 4(h)), with a minor role for the Nd-p electronic shell (Fig. 4(d)). The sharp peaks of ~ 1.87 and ~ 2.5 eV is responsible for the Nd-f electronic shell (Fig. 4(e)). They can observe the different curves of TDOS and PDOS due to the electronic Nd-4f shell for the NdFeSi compound. E_F is shown in Table 1. The TDOS and PDOS for the NdFeSi component demonstrate their metallic nature. Table 3 displays the calculated magnetic moments of the NdFeSi compound, as well as the magnetic moments of the interstitial region and individual atoms (Fe, Si). The individual moment of Nd3+ dominates the total magnetic moment of the NdFeSi compound. The Nd-4f electronic shell is responsible for the magnetic moment.

Table 3. Magnetic properties (μ_B) in of NdFeSi compound

	Spin magnetic moments μ_B
Interstitial region of magnetic moment	1.23229
Magnetic moment of Nd	3.40766
Magnetic moment of Fe	-0.51018
Magnetic moment of Si	-0.00057
Total Magnetic moment of NdFeSi	7.02610

Thermodynamic behavior

We are discussing thermal behaviour at a wide temperature and pressure, which gives us valuable information about the material. We determined the thermal behaviour by combining the GIBBS2 software with the WIEN2k software, which uses the Debye model. When the atoms of a crystal vibrate, it changes some of its thermodynamic properties inside the crystal, which also changes some of the thermodynamic parameters of the materials that we have observed. We looked at how heat behaves in terms of the Grüneisen parameter (γ), the bulk modulus (B_0), the Debye temperature (θ_D), and the entropy (S) at a range of temperatures and pressures. We used wide temperature (0–300 K) and pressure ranges (0–50 GPa) in the present research work to calculate all thermal parameters for NdFeSi. In a thermal system, entropy (S) is defined as energy and matter dispersal. This is also defined as the calculation of disorder for a system on a microscopic level. It is based on the compound NdFeSi temperature- and pressure-dependent parameters, as shown in Figs. 5(a) and 5(e), respectively. In Fig. 5(a), the vibration energy decreases as the temperature increases, causing the value of S to also decrease. The entropy (S) is mainly responsible for the vibrations in the atoms, resulting in the internal energy of the atomic orbital also increasing. Figure 5(e) illustrates the influence of pressure on entropy (S). When pressure rises, the material's entropy (S)
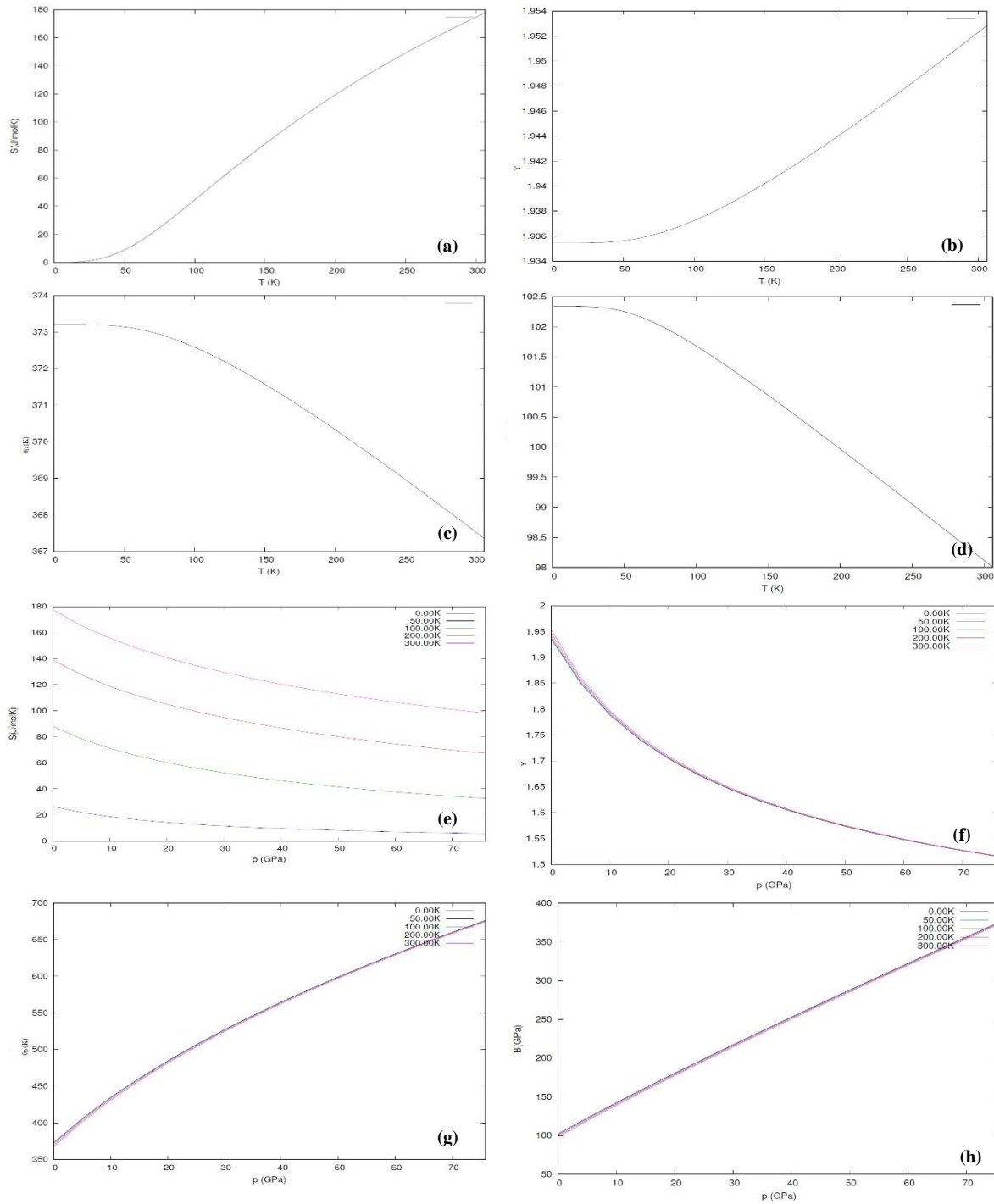
Fig. 5. (a) Variation in temperature Vs entropy *S*, (b) variation in temperature Vs the Grüneisen parameter *γ*, (c) variation in temperature Vs the Debye temperature θ$_D$, (d) variation in temperature Vs the bulk modulus *B*, and (e) variation in pressure Vs entropy *S*, (f) variation in pressure Vs the Grüneisen parameter *γ*, (g) variation in pressure Vs the Debye temperature θ$_D$, (h) variation in pressure Vs the bulk modulus *B*, for NdFeSi

decreases at a slow rate. Therefore, the volume of the unit cell decreases, and the internal energy of the material increases, resulting in reduced entropy (S). The effect of different temperatures on the Grüneisen parameter (*γ*) is shown in Fig. 5(b). The Grüneisen parameter is a function of the crystal lattice; it's defined as anharmonicity. Figure 5(b) indicates that the value of γ was found to be nonzero at *T* = 0 K, but when the temperature increases, the value of *γ* also increases. This shows that the anharmonicity of crystal lattices rises with

temperature. Figure 5(f) illustrates the effect of different pressures on γ. It has been found to decrease the value of γ when pressure is increased. As you can see in Fig. 5(c,g), the NdFeSi changes its Debye temperature (θ_D) at different temperature ranges (0–300 K) and pressure ranges (0–50 GPa). At T = 0 K, the value of θ_D is found at ~ 366.25 K. It is seen in Fig. 5. Figure 5(c) demonstrates that an increase in temperature leads to a decrease in the value. We are discussing thermal behaviour at a wide temperature and pressure, which gives us valuable information about the material. We determined the thermal behaviour by combining the GIBBS2 software with the WIEN2k software, which uses the Debye model. When the atoms of a crystal vibrate, it changes some of its thermodynamic properties inside the crystal, which also changes some of the thermodynamic parameters of the materials that we have observed. We looked at how heat behaves in terms of the Grüneisen parameter (γ), the bulk modulus (B_0), the Debye temperature (θ_D), and the entropy (*S*) at a range of temperatures and pressures. We have used wide temperature ranges (0–300 K) and pressure ranges (0–50 GPa) in our present research work to calculate all thermal parameters for NdFeSi. In a thermal system, entropy (*S*) is defined as energy and matter dispersal. This is also defined as the calculation of disorder for a system on a microscopic level. It is based on the compound NdFeSi's temperature- and pressure-dependent parameters, as shown in Fig. 5(a,e). In Fig. 5(a), the vibration energy decreases as the temperature increases, causing the value of S to also decrease. The entropy (*S*) is mainly responsible for the vibrations in the atoms, resulting in the internal energy of the atomic orbital also increasing. Figure 5(e) illustrates the influence of pressure on entropy (*S*). When pressure rises, the material's entropy (*S*) decreases at a slow rate. Therefore, the volume of the unit cell decreases, and the internal energy of the material increases, resulting in reduced entropy (*S*). The effect of different temperatures on the Grüneisen parameter (γ) is shown in Fig. 5(b). γ is a function of the crystal lattice; it's defined as anharmonicity. Figure 5(b) indicates that the value of γ was found to be nonzero at T = 0 K, but when the temperature increases, the value of γ also increases. This shows that the anharmonicity of crystal lattices rises with temperature. Figure 5(f) illustrates the effect of different pressures on γ. It has been found to decrease the value of γ when pressure is increased. As you can see in Fig. 5(c,g), the NdFeSi compound changes its Debye temperature (θ_D) at different temperature ranges (0–300 K) and pressure ranges (0–50 GPa). At T = 0 K, the value of θ_D is found at ~ 366.25 K. It is seen in Fig. 5. Figure 5(c) illustrates that an increase in temperature results in a decrease in the value of θ_D. decreases to ~ 50 K, and then the value of θ_D gradually decreases with the increase in temperature. However, when *T* exceeds 50 K, the temperature rapidly decreases the value of θ_D. The temperature decreases to approximately 50 K, after which the value of θ_D gradually decreases with an increase in temperature. However, when *T* exceeds 50 K, the temperature rapidly decreases the value of θ_D.

    Figure 5(g) illustrates the pressure's impact on the θ_D. In Table 3, we find the value of θ_D at 366 to 368 K at *P* = 0 with various temperature ranges (0–300 K). As a result, the value of θ_D also increases gradually with the increase in pressure. Another part of the NdFeSi compound's thermal behaviour is shown in Fig. 5(d,h), which show the bulk modulus (B_0) at different temperatures (0–300 K) and pressures (0–50 GPa). The value of B_0 offers details about the material, how it affects the degree of resistance (DOR) of materials, and how hard or soft the material is. At this point, when the compound

temperature increases, the degree of resistance decreases, and the compound becomes more flexible as the temperature rises. Figure 5(d) illustrates that an increase in temperature leads to a decrease in the value of B_0 for the NdFeSi compound, resulting in a change in its unit cells. At $T = 0$ K, the value of B_0 is found at ~ 40 GPa, but after $T = 40$ K, the value of B_0 decreases rapidly for the NdFeSi compound. Analysis of these results reveals that the B_0 changes with temperature, solely due to changes in the crystal's unit cell. Figure 5(h) illustrates the pressure's impact on the B_0. Table 3 finds the value of B_0 at approximately 96 to 98 GPa at $P = 0$, across various temperature ranges (0–300 K). As a result, the value of B_0 also increases gradually with the increase in pressure. As a result, the value of B_0 also increases slowly with the increase in pressure. The degree of resistance then rises, and our compound becomes inflexible (hard).

Conclusions

We have calculated the structural, electronic, magnetic, and thermal properties of the NdFeSi compound using the DFT method and the FPAPW+LO technique, with the assistance of WIEN2K software. We have investigated the structural and electronic properties of the NdFeSi material, obtaining information on the lattice constant, bulk modulus, a derivative of bulk modulus, band diagrams, and the total and partial density of states (TDOS and PDOS), respectively. In terms of electronic properties, our compound has a metallic nature because of the Nd-4f electronic shell. Similarly, the magnetic behaviour of the NdFeSi compound shows that the magnetic personality due to the Nd-4f electronic shell is responsible for its magnetic nature. A lot of different temperatures and pressures (0–50 GPa) were used to study the thermal behaviour of different materials. The Grüneisen parameter (γ), the bulk modulus (B_0), the Debye temperature (θ_D), and the entropy (S) were investigated. We have discussed the bulk modulus (B_0). As a result, when the temperature of the material increases, the material's softness also increases, but when the pressure of the material increases, the material's hardness also increases. In the case of Debye temperature (θ_D), pressure is more effective than temperature. As a result, the material's energy density increases, consuming a large amount of energy within a small space, leading to a decrease in the material's entropy (S).

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