Investigation on Structural, Elastic and Thermodynamic Properties of $MgNi_3$ Intermetallic Compound Using Density Functional Theory

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Magnesium based alloys belong to a class of materials, which have recently attracted great interest. In the present work, we report structural, elastic, and thermodynamic properties for the novel intermetallic compound $MgNi_3$ calculated using plane-wave pseudo potential (PW-PP) method within density functional theory (DFT), with local density approximation (LDA) and generalized gradient approximation (GGA). The comparison of the calculated equilibrium lattice constants and experimental data showed very good agreement for both approximations. The elastic constants were determined from a linear fit of the calculated stress-strain function according to Hooke's law. Once the elastic constants were obtained, the bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio σ anisotropy factor A, and the ratio B/G for $MgNi_3$ compound were deduced using Voigt-Reuss-Hill (VRH) approximation. Our calculated elastic constants indicate that the ground state structure of $MgNi_3$ is mechanically stable. The calculation results also show that this intermetallic crystal is stiff, elastically anisotropic, and ductile material. The Debye temperature is also predicted from elastic constants. The temperature dependence of the enthalpy H, free energy F, entropy S, and heat capacity at constant volume C_v of $MgNi_3$ crystal in a quasi-harmonic approximation are obtained from phonon density of states and discussed for the first report.

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1. Introduction

The technological application of magnesium alloys has been a hot research topic in recent years. In Mg-Ni binary alloy system a new phase $MgNi_3$ was formed by mechanical alloying in Mg-50 at % Ni mixture powders milled for 40 h [1]. The intermetallic compound $MgNi_3$ belongs of the family of magnesium alloys, where the research on magnesium (Mg) based alloys is of substantial interest due to its low density ($\sim$ 1.74 g/cm^3) and high specific strength and stiffness than many other engineering materials, including aluminium, steel, and polymer-based composites [2]. Magnesium alloys are among the lightweight engineering materials known and they are used in a variety of applications, particularly in automobile industry, aerospace manufacturing, and biomedical application [3, 4].

The motivation behind this work is the lack or at least the scarcity of bibliographic data on fundamental properties of the $MgNi_3$ compound and the above-mentioned features and important applications of magnesium based alloys. The main aim of this study is to investigate the physical properties such as structural, elastic, and thermodynamic properties of this new compound in magnesium-transition metal (Mg-Ni) system. Thus, in this work, we carried out a systematic theoretical investigation using first principle calculations which is one of the efficient ways to explore the structural, elastic, and thermodynamic properties of $MgNi_3$ alloy. This study was done, to provide data for further experimental and theoretical studies. The calculated results of this work were compared with available experimental and theoretical values, which could provide a theoretical guidance to design a new kind of magnesium alloy. The rest of this paper is organized as follows: the computational method is described in Sect. 2. The numerical results and discussions are given in Sect. 3, and finally, a conclusion is presented in Sect. 4.

2. Computational method

The structural, elastic and thermodynamic properties of the $MgNi_3$ intermetallic compound have been computed using the plane-wave pseudopotential method based on density functional theory (DFT) [5, 6], as implemented in the Cambridge Serial Total Energy Package (CASTEP) simulation program [7]. This is, in principle, an exact theory of the ground state. The exchange and correlation (XC) potential was generated within the local density approximation (LDA) developed by Ceperley and Adler and parameterized by Perdew and Zunger [8, 9], as well as within the generalized gradient approximation (GGA), with the functional of Perdew, Burke, and Ernzerhof, known as PBE [10]. The Coulomb potential energy caused by electron-ion interaction is described using the Vanderbilt-type ultrasoft scheme [11] in which, the orbitals of Mg ($2p^6 3s^2$),

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Ni ($3d^8 4s^2$) are treated as valence electrons. The cut-off energy for the plane-wave expansion was chosen at 340 eV and the Brillouin zone sampling was carried out using the $8 \times 8 \times 8$ set of Monkhorst-Pack mesh [12] from convergence tests.

The structural parameter (a) of $MgNi_3$ was determined using the Broyden–Fletcher–Goldfarb–Shenno (BFGS) minimization technique [13]. This method usually provides a fast way of finding the lowest energy structure.

In the structural optimization process, the energy change, maximum force, maximum stress, and maximum displacement are set at 1×10^{-5} eV/atom, 0.03 ev/Å, 0.05 GPa, and 0.001 Å, respectively.

The elastic constants were determined from first-principles calculations by applying a given homogeneous strain (deformation) with a finite value and calculations of the resulting stress according to Hook's law [14]. The total energy converged to 1×10^{-6} eV/atom in the self-consistent calculation.

3. Results and discussion

3.1. Structural properties

In Mg–Ni binary alloy system, a new phase $MgNi_3$ with the same crystal lattice as $AuCu_3$ phase was formed by mechanical alloying. $MgNi_3$ phase had the cubic crystal lattice and the equilibrium lattice parameter was determined to be $a = 3717$, with the space group $Pm3m$ (No 221) [1]. Nickel (Ni) atoms were located at the face-centred positions and Magnesium (Mg) atoms at the corners of the cubic unit cell. The unit cell structural model of the $MgNi_3$ compound is built according to the experimental data [1], as shown in Fig. 1. The crystal structure was optimized at first. The obtained results of calculated lattice parameter a of $MgNi_3$ intermetallic compound using the (PW-PP) method within both the LDA and the GGAPBE approximations are presented in Table I, together with experimental data for comparison. From the results presented in Table I, one can see that the calculated lattice constants are underestimated by LDA and GGA-PBE approximations. It is 4.11% smaller than the experimental value using LDA and it is only 140% smaller than the experimental value using GGAPBE. We can say that our calculated equilibrium lattice parameters agree well with the experimental data in both approximations.

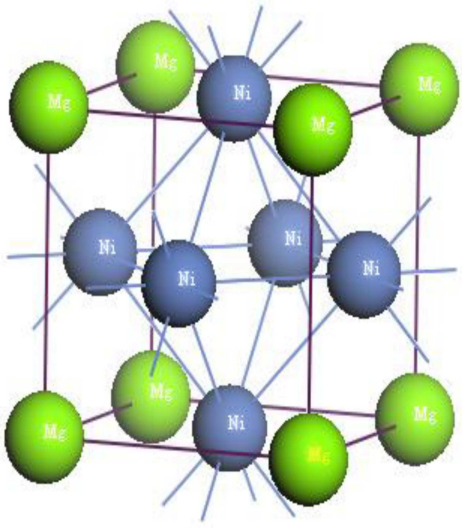

Fig. 1. The cubic crystal structure of $MgNi_3$ intermetallic compound.

TABLE I

Calculated and experimental values of the equilibrium lattice constant a, the volume, the enthalpy of formation ΔH, the bulk modulus B and its pressure derivative B' of $MgNi_3$ compound.

	LDA	GGA	Experiment [1]
a [Å]	3.564	3.665	3.717
V [Å^3]	45.270	49.229	51.35
ΔH [eV]	−06.92	−05.98	–
B [GPa]	169.90	135.42	–
B'	4.65	4.48	–

The total energies are calculated in both LDA and GGA-PBE for approximations the $MgNi_3$ intermetallic compound for different volumes around the equilibrium cell volume V. The plots of calculated total energies versus reduced volume for this compound in both approximations are illustrated in Fig. 2a and b. Then, the curves of the total energies as a function of the volume are fitted to the Murnaghan's equation of state [15] to obtain the ground state properties such as the bulk modulus B and its pressure derivative B'. The results obtained for these parameters (B, B') in the two approximations LDA and GGA-PBE are given in Table I. We think no previous calculations match as well with the experimental data for comparison.

The formation enthalpy ΔH at zero temperature is calculated, in order to estimate the thermal stability of the $MgNi_3$ intermetallic, as follows

$$\Delta H = \frac{E_{\text{tot}} - N_{\text{Mg}} E_{\text{Mg}} - N_{\text{Ni}} E_{\text{Ni}}}{N_{\text{Mg}} + N_{\text{Ni}}}. \quad (1)$$

Here E_{tot} represents the total energy of unit cell. E_{Mg} and E_{Ni} are electronic total energy per atom for pure Mg and Ni in ground state, respectively. N_{Mg} and N_{Ni} are the number of composition elements in unit cell, respectively [16]. The result obtained from the calculation is listed in Table I. The negative enthalpy of formation indicates that the ground state of this compound is thermodynamically stable.

3.2. Elastic and mechanical properties

The elastic properties are the most basic properties to reflect the essential interactions between atoms of materials. Such properties provide very important information about the binding characteristic in-between the adjacent planes of atoms, the anisotropic

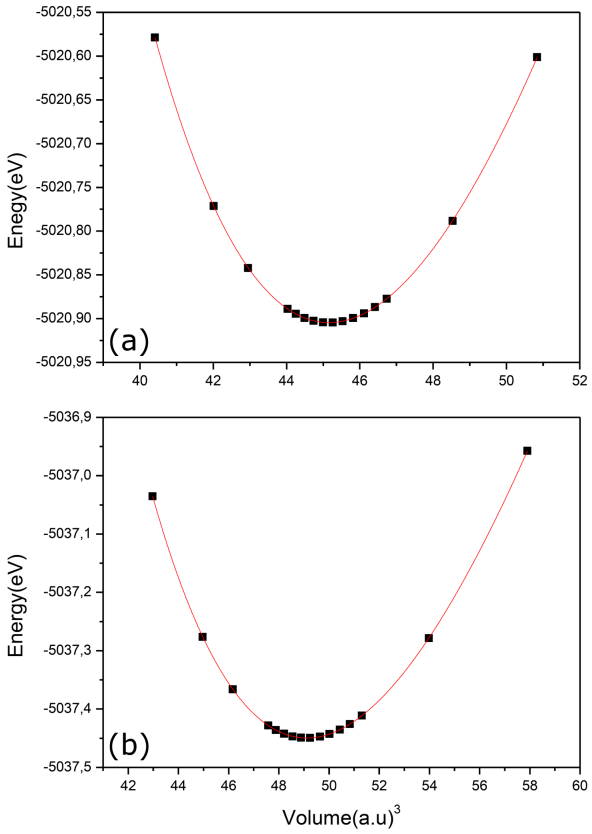

Fig. 2. Total energy versus cell volume using (a) local density approximation (LDA), and (b) generalized gradient approximation (GGA).

character of binding, and the stability of the structure. The elasticity of a cubic crystal is specified by the three independent elastic constants C_{11}, C_{12}, and C_{44}. In this work, the calculated elastic constants of $MgNi_3$ compound at zero pressure and temperature are presented in Table II. For a cubic crystal, the obtained elastic constants meet the requirements of mechanical stability criteria: $C_{11} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{11} + 2C_{12} > 0$, and $C_{11} > B > C_{12}$. From Table II, one can see that the elastic constants of $MgNi_3$ compound satisfy all of these conditions, suggesting that the structure of $MgNi_3$ is mechanically stable at ambient condition. The elastic constants values calculated with the LDA approximation are slightly higher than those obtained using the GGA–PBE approximation. So far, there are no experimental and other theoretical data available in literature for the elastic constants (C_{ij}) of $MgNi_3$ for comparison, so we consider our present results as predictions which still await an experimental confirmation.

The most important parameters for estimating mechanical properties of materials such as bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio (σ) are obtained from results of the calculated single-crystal elastic constants C_{ij} using

TABLE II

The Calculated values of the elastic constants C_{ij}, bulk modulus B, shear modulus G, Young's modulus E, Poisson's ratio σ, anisotropy factor A, and B/G in cubic structure of $MgNi_3$ compound.

	LDA	GGA
C_{11} [GPa]	218.08	181.51
C_{12} [GPa]	143.39	118.69
C_{44} [GPa]	107.82	90.04
B [GPa]	168.29	139.63
G [GPa]	70.54	59.06
E [GPa]	185.68	155.29
σ	0.32	0.31
A	2.89	2.87
B/G	2.39	2.36
H [GPa]	8.44	7.51

the Voigt-Reuss-Hill (VRH) averaging scheme [17]. The Voigt–Reuss–Hill approximation gives the effective values of the bulk and shear moduli. For the cubic system, the Voigt bounds [18] of the bulk modulus B_{V} and shear modulus G_{V} are given by the relations

$$B_{\mathrm{V}} = \frac{(C_{11} + 2C_{12})}{3}, \tag{2}$$

and

$$G_{\mathrm{V}} = \frac{(C_{11} - C_{12} + 3C_{44})}{5}. \tag{3}$$

The Reuss bounds [19] of the bulk and shear moduli are given by the relation $B_{\mathrm{R}} = B_{\mathrm{V}}$ and

$$G_{\mathrm{R}} = \frac{5C_{44}\,(C_{11} - C_{12})}{4C_{44} + 3\,(C_{11} - C_{12})}. \tag{4}$$

Finally, the bulk modulus B and shear modulus G, based on Hill approximation are arithmetic average of Voigt and Reuss elastic moduli, and they are expressed as

$$B = \frac{1}{2}\,(B_{\mathrm{V}} + B_{\mathrm{R}})\,, \tag{5}$$

and

$$G = \frac{1}{2}\,(G_{\mathrm{V}} + G_{\mathrm{R}})\,. \tag{6}$$

Young's modulus (E) and Poisson's ratio (σ) can be calculated by using Hill's elastic moduli (B) and (G), which are given as

$$E = \frac{9BG}{3B + G}, \tag{7}$$

$$\sigma = \frac{3B - 2G}{2\,(3B + G)}. \tag{8}$$

The calculated results for these moduli and Poisson's ratio for the $MgNi_3$ compound are listed in Table II. The bulk modulus is usually assumed to be a measure of resistance to volume change by applied pressure. From Table II, it can be seen that the value of the bulk modulus of $MgNi_3$ compound is larger, indicating that it has a strong resistance to volume change by applied pressure. The calculated values of the bulk modulus B

from the elastic constants, using LDA and GGA have nearly the same values as the ones obtained from the fit to a Birch–Murnaghan EOS (B). This might be an estimate of the reliability and accuracy of our calculation. The two constants E and G are all that are needed to fully characterize the stiffness of an isotropic material. The present calculations for these moduli demonstrate that the $MgNi_3$ compound is stiff. The Poisson's ratio (σ), defined as the ratio of transverse strain to the longitudinal strain, is used to reflect the stability of the material against shear and provides information about the nature of the bonding forces. It takes the value $-1 < \sigma < 1/2$. No real material is known to have a negative value of σ. So this inequality can be replaced with $0 < \sigma < 1/2$. The low value of Poisson's ratio indicates a large compression of volume and when $\sigma = 0.5$ no volume change occurs. The bigger the Poisson's ratio is, the better the plasticity is. The present calculation for the Poisson's ratio shows that the $MgNi_3$ intermetallic compound possesses good plasticity.

The Zener anisotropy factor (A) is a measure of the degree of anisotropy in solid [20]. It takes the value of 1 for an isotropic material. It provides a measure of the degree of elastic anisotropy, when the A values are smaller or greater than unity. The Zener anisotropy factor (A) of $MgNi_3$ compound is calculated by the following equation

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \tag{9}$$

As shown in Table I, the calculated Zener anisotropy factor A is larger than 1 for both approximations LDA and GGA, which indicates that the $MgNi_3$ compound is anisotropic material.

The ratio B/G is a simple relationship related to brittle or ductile behaviour of materials. It has been proposed by Pugh [21]. A high B/G ratio is associated with ductility, whereas a low value corresponds to the brittleness. The critical value separating ductile and brittle material is 1.75. The calculated results are listed in Table II. In this work, the obtained results of both approximations LDA and GGA indicate that $MgNi_3$ compound can be classified as ductile material at zero pressure. Another parameter indicating the brittleness or ductility of the material is the Cauchy relation defined as $C_P = C_{12} - C_{44}$. The material is expected to be ductile, if the value of this expression is positive. On the other hand, if its value is negative, the material is brittle [22]. At zero pressure, we found 3557 GPa and 2865 GPa for Cauchy pressure within both LDA and GGA approximations, respectively. From these values and according to above criterion, the studied compound is ductile. Thus, the ductile nature of $MgNi_3$ compound can be related to the metallic character in its bonds.

In addition, the hardness is also one fundamental physical parameter when considering the mechanical properties of polycrystalline $MgNi_3$ intermetallic. The theoretical hardness parameter (H) denoting the resistance of the physical object against compression of the contacting parts is applied [23]. So here we calculate the hardness of $MgNi_3$ by using the approach as expressed below

$$H = \frac{E}{6}\frac{(1-2\sigma)}{(1+\sigma)}. \tag{10}$$

The hardness associated to this polycrystalline intermetallic crystal in both approximations LDA and GGA-WC are listed in Table II. It can be seen that $MgNi_3$ compound has a low hardness. It turns out that the $MgNi_3$ compound is a low stiff material. The low hardness of this crystal can be attributed to the low density of crystal structure.

3.3. Thermodynamic properties

The Debye temperature (Θ_{D}) corresponds in the Debye theory to a maximum phonon frequency. It reflects the structural stability, the strength of bonds, and it is closely related to many physical properties such as specific heat and melting temperature. At low temperature the Debye temperature calculated from elastic constants is the same as that determined from specific heat measurements. One of the standard methods to calculate the Debye temperature (Θ_{D}) is from elastic data, since Θ_{D} may be estimated from the average sound velocity v_m by the following expression [24]:

$$\Theta_{\mathrm{D}} = \frac{h}{k_{\mathrm{B}}}\left(\frac{3}{4\pi}\frac{n}{V_a}\right)^{\frac{1}{3}} v_m, \tag{11}$$

where h is Plank's constant, k_{B} is Boltzmann's constant, n is the number of atoms per formula unit, and V_a is the atomic volume. The average sound velocity in the polycrystalline material is given by the following equation [25]:

$$v_m = \left[\frac{1}{3}\left(\frac{1}{v_l^3} + \frac{2}{v_t^3}\right)\right]^{-\frac{1}{3}}, \tag{12}$$

where v_l and v_t are the longitudinal and transverse sound velocities of an isotropic aggregate, obtained using the shear modulus G and the bulk modulus B from Navier's equation [26]:

$$v_l = \left(\frac{3B + 4G}{3\rho}\right)^{1/2}, \tag{13}$$

$$\text{and } v_t = \left(\frac{G}{\rho}\right)^{1/2}. \tag{14}$$

The calculated Debye temperature (Θ_{D}) and sound velocities (v_m, v_l, v_t) as well as the density (ρ) for $MgNi_3$ compound in both approximations LDA and GGA are listed in Table III. Unfortunately, there are no experimental and other theoretical data for comparison. So we consider the present results of Debye temperature (Θ_{D}) as a prediction for the first time, which still awaits an experimental confirmation.

Phonons are an important concept in solid state physics, which provides access to a wide range of important properties such as phase stability, specific heat, thermal expansion, heat conduction, and phase transformations. In Fig. 3, we display the calculated total

TABLE III

Density (ρ), longitudinal, transverse and average sound velocities (v_l, v_t and v_m), and the Debye temperature (Θ_{D}) of the $MgNi_3$ compound.

	LDA	GGA	Experiment [1]
ρ [g cm^{-3}]	7.35	6.76	6.48
ν_l [m s^{-1}]	5974.36	5863.68	–
ν_t [m s^{-1}]	3097.95	2955.79	–
ν_m [m s^{-1}]	3467.49	3314.25	–
Θ_{D} [K]	459.84	427.42	–

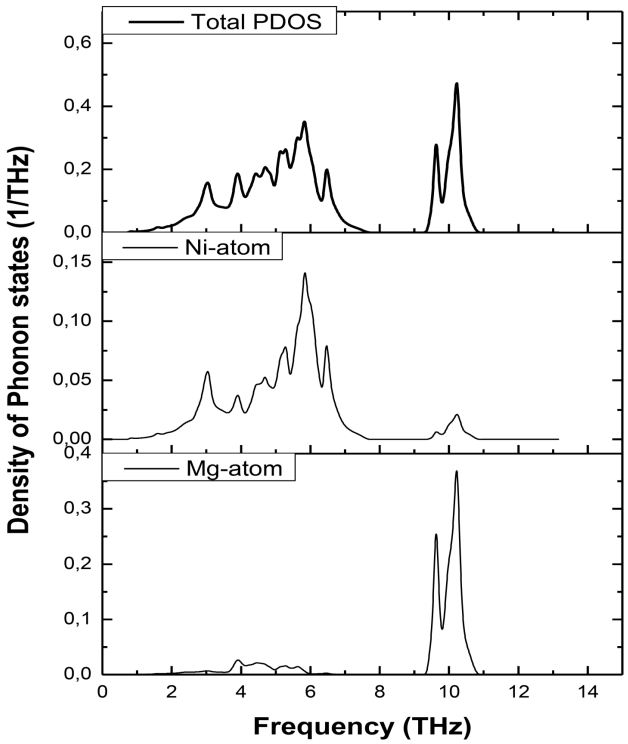

Fig. 3. Total phonon density of states (PDOS) and partial phonon DOS of constituent atoms of $MgNi_3$ compound.

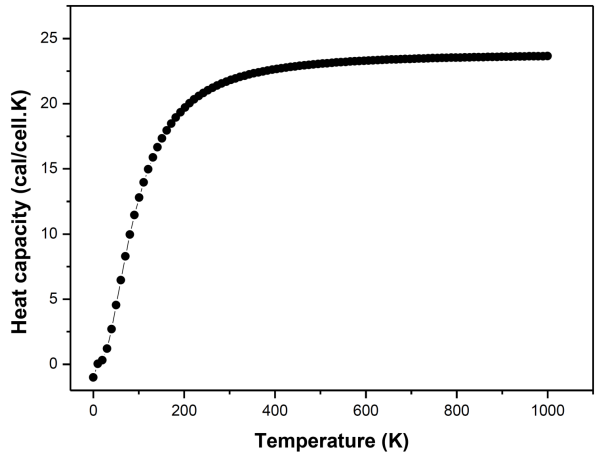

Fig. 4. Heat capacity at constant volume C_v as a function of temperature.

phonon density of states (PDOS) for $MgNi_3$ compound along with some high symmetry directions in the Brillouin zone (BZ), together with the separate contributions of Mg and Ni vibrations. As shown in Fig. 3, the results indicate that the phonon structure is stable since throughout the Brillouin zone all phonon frequencies are positive. Moreover the phonon density of states can be viewed as two bands. One is the band lower than 8 THz where the main contribution comes from Ni atoms, while the other is the band higher than 9 THz where the contribution comes from Mg atoms.

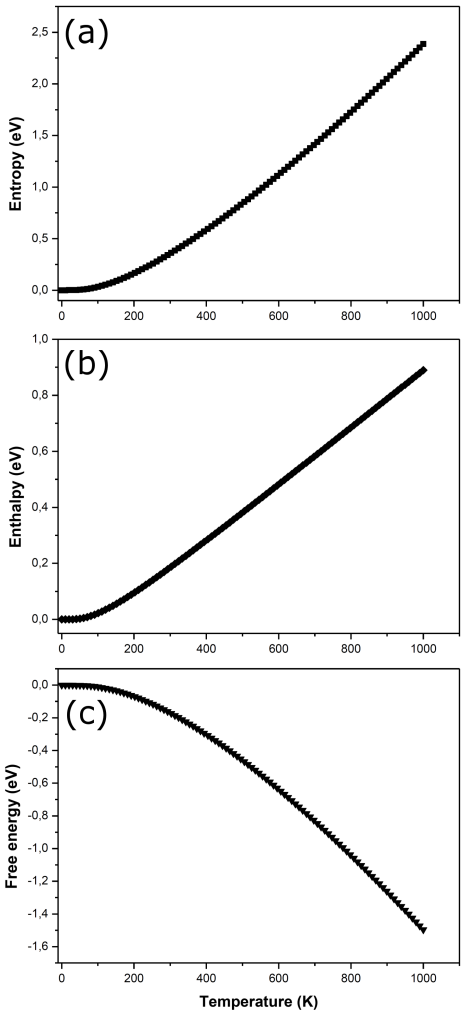

Fig. 5. Temperature dependence of (a) the entropy, (b) the enthalpy, and (c) the free energy.

The thermodynamic properties of the present material such as the heat capacity C_v at constant volume, the entropy S enthalpy H, and free energy F in a quasi-harmonic Debye approximation are evaluated using calculations for the phonon density of states (PDOS). In this work, the phonon contribution to the specific heat C_v, to the entropy S, to enthalpy H, and to free energy F, as a function of temperature for $MgNi_3$ intermetallic compound, are shown in Fig. 4 and Fig. 5(a–c),

respectively. The calculated value of zero point energy at 0 GPa is 0.15 eV. At ambient temperature, the heat capacity C_v is 21.75 Cal/(Cell K) and it tend to the asymptotic limit (so called the Dulong–Petit limit) of $C_v = 23.64$ Cal/(Cell K) $= 3$ nN k_B at higher temperatures, as shown in Fig. 4. From Fig. 5a and b, we can see that the entropy S and the enthalpy H increase continually as temperature increases, while the free energy (Fig. 5c) decreases gradually with increasing temperature. As the temperature of the crystal increases the particle vibrates more vigorously, causing an increase in entropy of the system. The experimental thermodynamic data of $MgNi_3$ cannot be found. Therefore it is difficult to evaluate the magnitude of errors between theory and experiment. Our calculated results can be seen as a prediction for future investigations.

3.4. Electronic properties

The study of electronic properties allows us to determine the type of the compound (metal, insulator, or semiconductor) as well as chemical bonding. The electronic structure properties of this compound are calculated along high symmetry directions in the Brillouin zone using the local density approximation. The obtained electronic band structure is shown in Fig. 6. It is clear from the band graph that the valence and conduction bands overlap each other and there is no band gap at the Fermi level E_F, which confirms the metallic nature of this intermetallic compound. The total density of states (TDOS) and partial density of states (PDOS) are shown in Figs. 7 and 8. In Fig. 7, *d*-states show the main contribution in TDOS plot near Fermi level.

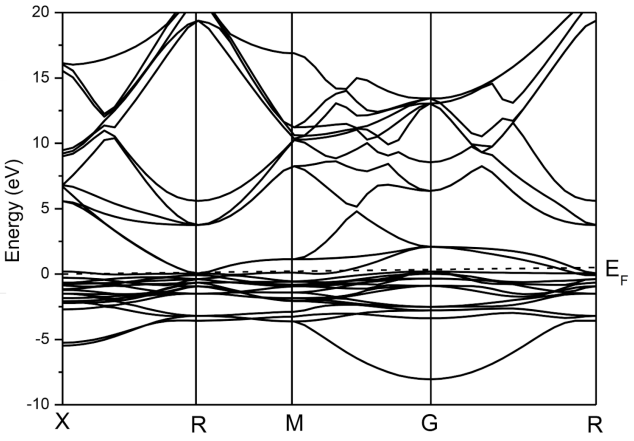

Fig. 6. Band structure with Fermi energy level E_F of $MgNi_3$.

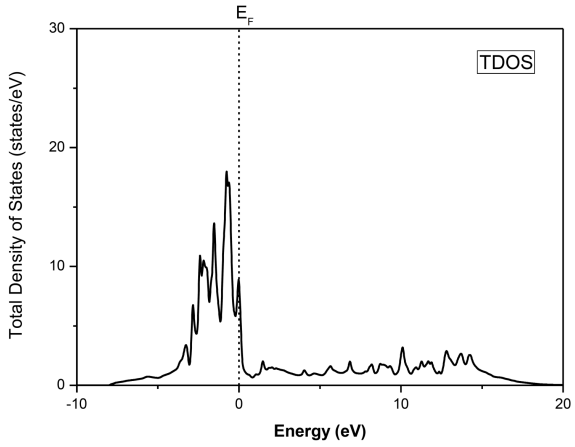

Fig. 7. Total density of states of $MgNi_3$.

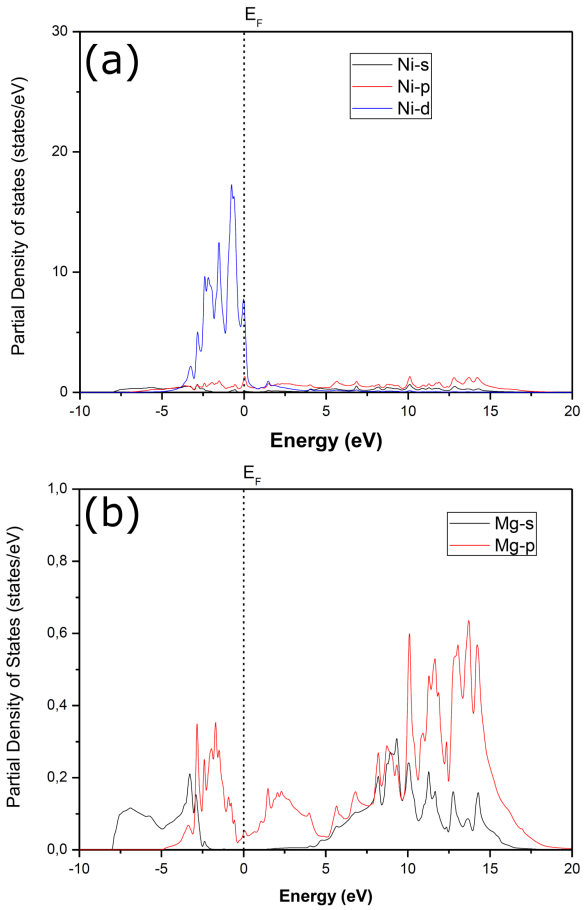

Fig. 8. Partial density of states of (a) Ni atoms and of (b) Mg atom are obtained for $MgNi_3$.

4. Conclusions

The present theoretical study investigated the structural, elastic, mechanical, and thermodynamic properties of $MgNi_3$ intermetallic compound by means of the DFT within LDA and GGA approximations. Our results for the optimized lattice parameter (a) are in good agreement with the available experimental data. The elastic constants C_{ij}, and related polycrystalline mechanical parameters such as bulk modulus B, shear modulus G, Young's modulus E, and Poisson coefficient σ are calculated. The $MgNi_3$ compound is mechanically

stable according to the elastic stability criteria, while no experimental results of elastic moduli are available for comparison. The Zener factor A, the B/G ratio and Cauchy pressure $(C_{12} - C_{44})$ are also estimated. The calculated Zener factor indicates that $MgNi_3$ compound is elastically anisotropic. The values of the ratio B/G and Cauchy pressure show a ductile manner for the $MgNi_3$ compound. Finally, from the knowledge of the elastic constants and the average sound velocities and using the quasi-harmonic Debye model, the calculated PDOS the thermodynamic properties have been predicted successfully. The heat capacity at constant volume of $MgNi_3$ increases sharply with temperature at low temperature and it tends to Dulong-Petit limit at high temperature. The structure band and density of states show that the $MgNi_3$ compound exhibit metallic properties.

Acknowledgments

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References

[1] G. Liu, S. Xi, G. Ran, K. Zuo, P. Li, J. Zhou, *J. Alloys Comp.* **448**, 206 (2008).

[2] C.X. Shi, *J. Magnes. Alloy.* **1**, 1 (2013).

[3] K.U. Kainer, *Magnesium-Alloys and Technology*, Wiley-VCH, Weinheim, 2003.

[4] N. Li, Y. Zheng, *J. Mater. Sci. Technol.* **29**, 489 (2013).

[5] P. Hohenberg, W. Kohn, *Phys. Rev. B* **136**, 864 (1964).

[6] W. Kohn, L.J. Sham, *Phys. Rev. A* **140**, 113 (1965).

[7] M.D. Segall, P.J.D. Lindan, M.J. Probert, C.J. Pickard, P.J. Hasnip S.J. Clark, M.C. Payne, *J. Phys. Condens. Matter* **14**, 2717 (2002).

[8] D.M. Ceperley, B.J. Alder, *Phys. Rev. Lett.* **45**, 566 (1980).

[9] J.P. Perdew, A. Zunger, *Phys. Rev. B* **23**, 5048 (1981).

[10] J.P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).

[11] D. Vanderbilt, *Phys. Rev. B* **41**, 7892 (1990).

[12] H.J. Monkhorst, J.D. Pack, *Phys. Rev. B* **13**, 5188 (1976).

[13] T.H. Fischer, J. Almlof, *J. Phys.Chem.* **96**, 9768 (1992).

[14] J.F. Nye, *Propriétés Physiques des Matériaux*, Dunod, Paris, 1961.

[15] F.D. Murnaghan, *Proc. Natl. Acad. Sci. USA* **30**, 244 (1944).

[16] D.H. Wu, H.C. Wang, L.T. Wei, R.K. Pan, B.Y. Tang, *J. Magnes. Alloy.* **2**, 165 (2014).

[17] R. Hill, *Proc. Phys. Soc., London, Sect. A* **65**, 349 (1952).

[18] W. Voigt, *Lehrbuch de Kristallphysik (Terubner)*, Leipzig 1928.

[19] A. Reuss, Z. Angew, *Math. Mech.* **9**, 49 (1929).

[20] C. Zener, *Elasticity and Anelasticity of Metals*, University of Chicago Press, Chicago 1948.

[21] S.F. Pugh, *Philos. Mag.* **45**, 823 (1954).

[22] D.G. Pettifor, *Mater. Sci. Technol.* **8**, 345 (1992).

[23] H.C. Cheng, C.F. Yu, W.H. Chen, *J. Alloys Comp.* **546**, 286 (2013).

[24] P. Wachter, M. Filzmoser, J. Rebisant, *J. Physica B* **293**, 199 (2001).

[25] O.L. Anderson, *J. Phys. Chem. Solids* **24**, 909 (1963).

[26] E. Schreiber, O.L. Anderson, N. Soga, *Elastic Constants and their Measurements*, McGraw-Hill, New York 1973.