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First Principles Study on Structural, Electronic, Elastic and Thermal Properties of Equiatomic MTi (M = Fe, Co, Ni)

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Abstract
We have investigated the structural, electronic, elastic and thermal properties of MTi (M = Fe, Co and Ni) using *ab-initio* full potential linearized augmented plane wave (FP-LAPW) method within generalized gradient approximation (GGA) and local spin density approximation (LSDA). We have calculated the ground state and electronic properties such as lattice constant (a_0), bulk modulus (B), pressure derivative of bulk modulus (B') and density of states at Fermi level N(E_F) which are in good agreement with experimental and available other theoretical results. The elastic constants (C_{11}, C_{12} and C_{44}) and mechanical properties such as Poisson's ratio (σ), Young's modulus (E), shear modulus (G_H), anisotropic factor (A) are also calculated which are agree well with the experimental and other theoretical results. Ductility for these compounds have been analyzed by Pugh's rule (B/G_H ratio) and Cauchy pressure (C_{12} - C_{44}). Our calculated results reveals that NiTi is most ductile amongst the MTi (M = Fe, Co and Ni) compounds.
Keywords: Ab-initio, electronic properties, elastic properties, thermal properties.

1. Introduction

Intermetallics are short and summarizing designation for the intermetallic phases and compounds which result from the combination of various metals and form numerous and manifold class of materials. Much of change in character of intermetallic compounds is due to difference in the chemical bonding that binds the atoms of phase together. Intermetallic compounds have emerged as materials with vast potential for application in a wide range of technologically important areas [1]. The enormous potential of intermetallics especially aluminides stems from their many attractive properties, such as high oxidation, corrosion resistance and relatively low densities, combined with their ability to retain strength and stiffness at elevated temperatures [2, 3]. Their physical, electrical, magnetic and mechanical properties are often superior to those of ordinary metals, but their enormous potential to improve engineering performance remains largely unused because they are brittle and fracture easily at room temperature. Due to long range ordering and specific properties, the intermetallic alloys are assumed to fill an existing gap between structural ceramics and classical metallic alloys [4].

The intermetallic compounds of titanium FeTi, CoTi and NiTi have many interesting properties such as high hardness, melting temperature, shape memory effect, hydrogen capacity per unit weight etc. [5]. These intermetallic compounds of VIII- group element have unique functional and structural properties also. CsCl-type (B_2-phase) equiatomic alloys generally have low ductility at low temperatures in spite of relatively simple crystal structure. In particular NiAl and FeAl have high phase stability and exhibit poor ductility at room temperature [6]. NiTi is well known as shape memory alloy and super elastic material, while FeTi, CoTi are possible to be used as hydrogen storage materials. CoTi is also known to exhibit positive temperature dependence of yield strength [6]. In the last few years, the scientific investigations for NiTi have been made extensively from the aspects of theory and experiments, including the structural, thermodynamic and martensitic (B19') transformation path etc. [7]. Recently, spectroscopic ellipsometry study of FeTi, CoTi and NiTi alloys have revealed strong optical transitions and has explained the similarities and differences among optical conductivity spectra and measured results are much closer to those obtained by full potential linearized augmented plane wave (FP-LAPW) method [8]. Other studies were devoted to the role of structural disorder and magnetic properties in CoTi alloys and films [9]. Despite the technological importance of shape memory material and recent advances the fundamental mechanisms, that governs their unique behavior are not fully known, while the martensitic transformation governing the thermo-mechanical response of this material (NiTi) at the macroscale is well known characterized [10]. Kibey *et al.* [11] have presented energy landscape for martensitic phase transformation in shape memory NiTi using first principles calculation. Cheng *et al.* [12] have been carried out to study the elastic properties and electronic structure of NiTi, CoTi and FeTi using first principles calculations. Naish *et al.* [13] have theoretically analyzed possible martensitic phases in the NiTi. Kellou *et al.* [14] have reported the electronic properties, bulk surfaces and interfaces of FeTi, CoTi and NiTi alloys using FP-LAPW method. Zhao *et al.* [7] have investigated the structural and elastic properties, phase diagram of NiTi alloy from first principles calculations. The magnetic and electronic properties of CoTi alloys using LMTO method has been studied by Napierala *et al.* [15]. Eibler *et al.* [16] have reported the electronic, structure, chemical bonding

and spectral properties of FeTi, CoTi and NiTi using self-consistent APW method. Sheng *et al.* [17] investigated first principles calculation of intermetallic compounds in FeTiCoNiVCrMnCuAl systems high entropy alloy using CASTEP code.

In the present work, we have performed a first principles spin polarized calculation of FeTi, CoTi and NiTi, which crystallize in CsCl-type structure, using density functional theory (DFT) within the both generalized gradient approximation (GGA) and local spin density approximation (LSDA). We have also calculated the ductility of MTi (M = Fe, Co, Ni) by B/G_H ratio and Cauchy's pressure and found that all the compounds are ductile in nature. To the best of our knowledge the thermal properties are reported by us for the first time. We have also done a comparative study of their structural, electronic, elastic and mechanical properties.

2. Methodology

The first principles calculation of the real material based on the density functional theory is one of the most powerful tool to understand the electronic structure of these materials. It can give us the information about spin distribution in magnetic materials which are not measured from experiment. The total energy, ground state properties and electronic band structures have been computed in spin polarized calculation within GGA and LSDA approximations using full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [18]. Generalized gradient approximation (GGA) has been used for the exchange and correlation effects [19]. The energy eigen value convergence has been achieved by expanding the basis function up to $R_{MT}*K_{max}= 7$, where R_{MT} is the smallest atomic sphere radius in the unit cell and K_{max} gives the magnitude of the largest **k** vector in the plane wave expansion. The valence wave functions inside the spheres are expanded up to $l_{max} = 10$ while the charge density is Fourier expanded up to $G_{max} = 12$. The self consistent calculations are considered to converge when the total energy of the system is stable within 10^{-4} Ry. Energy to separate core and valence state is -6.0 R_y. Integrations in the Brillouin zone were performed using **k**-points generated with 10×10×10 mesh grids for all structures.

The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants namely C_{11}, C_{12} and C_{44}. Hence, a set of three equations is needed to determine all the constants. The first equation involves calculation of bulk modulus (B), which is related to the elastic constants as:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{1}$$

The second step involves volume-conservative tetragonal strain given by the following tensor:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \dfrac{1}{(1+\delta)^2} - 1 \end{bmatrix} \tag{2}$$

where $\delta = (1+e)^{-1/3}-1$ with e as strain tensor. Application of this strain has an effect on the total energy from its unstrained value as follows:

$$E(\delta) = E(0) + 3(C_{11} - C_{12}) + V_0\delta^2 + O(\delta^3) \tag{3}$$

where V_0 is the volume of the unit cell.

Finally, for the last type of deformation, we use in the volume-conserving rhombohedra strain tensor given by:

$$\frac{\delta}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{4}$$

which transforms the total energy to

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + O(\delta^3) \tag{5}$$

The thermal loss mechanisms (temperature dependence) of a material is most suitably described in terms of the Debye temperature (θ_D) which is a fundamental parameter closely related to many physical properties such as elastic constants, specific heat and melting temperature etc. One of the standard methods is to calculate the Debye temperature from elastic constants data, since θ_D may be estimated from the average sound velocity v_m by the following equation [20, 21]:

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi V_a}\right]^{1/3} v_m \qquad (6)$$

where h is Plank's constant, k_B is Boltzmann's constant, V_a is the atomic volume, n is the number of atoms per formula unit and v_m is average sound velocity. The average sound velocity is approximately calculated from [20, 22].

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \qquad (7)$$

where v_t and v_l are the transverse and longitudinal sound velocities respectively obtained by using the elastic constants as follows:

$$v_l = \sqrt{\frac{\left[C_{11} + \frac{2}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \qquad (8)$$

$$v_t = \sqrt{\frac{\left[C_{44} - \frac{1}{5}(2C_{44} + C_{12} - C_{11})\right]}{\rho}} \qquad (9)$$

where C_{11}, C_{12} and C_{44} are second order elastic constants and ρ is mass density per unit volume.

3. Result And Discussion

3.1 Structural Properties

The spin polarized calculations are carried out to obtain the total energy of (FeTi, CoTi and NiTi) intermetallic compounds using FP-LAPW method within GGA approximation. The variation of total energy as a function of volume has been plotted in Fig. 1 (a – c).

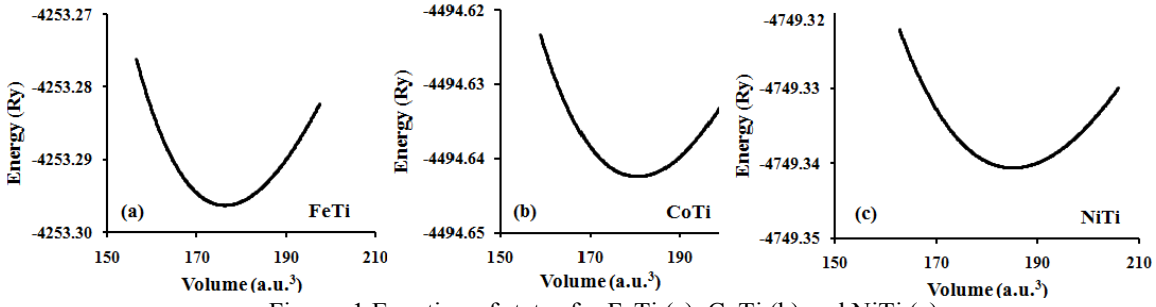

Figure. 1 Equation of states for FeTi (a), CoTi (b) and NiTi (c).

Table 1: Calculated ground state properties for MTi (M = Fe, Co and Ni).

Solids	Approximation	a_0 (Å)	B (GPa)	B'	$N(E_F)$
FeTi Pre.	GGA	2.96	182.38	5.44	0.16
	LSDA	2.90	235.10	4.34	0.19
Expt.		2.97			
Theo.		2.88[a]	192[a]		0.19[b]
			188[c]		
CoTi Pre.	GGA	2.99	173.56	3.96	1.51
	LSDA	2.91	180.89	4.41	1.30
Expt.		2.99[a]	152[a]		1.66[b]
Theo.		2.98[a]	204[a]		
NiTi Pre.	GGA	3.01	160.03	4.15	1.57
	LSDA	2.94	194.47	4.77	1.51
Expt.		3.01[a]	142[a]		1.73[b]
Theo.		2.99[a]	191[a]		

[a]:Ref[12] [b]:Ref[5] [c]:Ref[17]

In order to calculate the ground state properties of these intermetallics, the total energies are calculated in B_2 phase for different volumes. The calculated total energies are fitted to Birch Murnaghan's equation of state [23]

to determine the ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') at minimum equilibrium volume V_0.

$$E(V) = E_0 + \frac{BV}{B'}\left[\frac{(V_0/V)^{B'}}{(B'-1)} + 1\right] - \frac{BV}{B'-1} \tag{10}$$

Pressure is obtained by taking volume derivative of the total energy

$$P(V) = \frac{B}{B'}\left[\left(\frac{V}{V_0}\right)^{B'} - 1\right] \tag{11}$$

The ground state properties are presented in Table 1, and compared with other experimental and theoretical results. Our calculated bulk modulus (B) slightly differs with the other results reported in the literature which may be due to the different exchange correlation schemes. To the best of our knowledge the experimental bulk modulus of FeTi is not reported yet. The order of energetic stability of FeTi, CoTi and NiTi from high to low is : FeTi > CoTi > NiTi.

3.2 Electronic properties

The calculated band structure of FeTi, CoTi and NiTi intermetallic compounds using FP-LAPW method within GGA are presented in Fig. 2 (a, b and c) where Fermi level (E_F) is considered at origin. To further understand the nature of electronic bands structure, we have also calculate the total and partial density of states for these compounds at ambient pressure and presented in Fig. 3 (a - f). We found similar band profile in both GGA and LSDA for MTi (M = Fe, Co, Ni) compounds. We therefore present here the band structures in only GGA. In case of FeTi, the lowest lying bands around -7.4 eV at Γ-point are mainly due to '*s'* states of Fe. The bands above this and below the Fermi level (E_F) around -1.8 eV and -2.2 eV are due to hybridized '*d'* states of Fe and Ti. It can be noted from Fig. 2 (a) and 3 (a) that here two bands are crossing the Fermi level at X point which are mainly due to '*d'* states of Fe and Ti. It is seen from the Fig. 2 (a) that FeTi is metallic in nature due to strong hybridization '*d'* states of Fe and Ti. It is also seen from Fig. 3 (a) the number of DOS at Fermi level N (E_F) is 0.16 States/eV (Table 1). In Fig .2 (b) for CoTi the lowest lying band around -7.8 eV at Γ- point are mainly due to Co *'s'* like states and the bands above this and below the Fermi level around -2.2 eV and -2.8 eV are due to '*d'* states of Fe and Ti. The bands above the Fermi level are due to Ti '*d'* states. From Fig. 3 (c ,d) the hybridization between Co '*d'* and Ti '*d'* states from lowest band upto above the Fermi level can also be seen. The finite DOS at Fermi level N (E_F) are found to be 1.51 States/eV for GGA respectively (Table 1).

Similarly, in case of NiTi the lowest lying bands around -7.8 eV at Γ -point are mainly due to Ni *'s'* states and The cluster of bands just below the Fermi level (E_F) around -2.1 eV and -2.7 eV are due to mainly '*d'* states of Fe and Ti. It is also seen from Fig. 3(e, f) that there is strong hybridization between Ni-*d* and Ti-*d* states. The number of density of states at Fermi level N (E_F) is found to be 1.57 States/eV (Table. 1). From the analysis of band structure of these compounds it is observed that all the three compounds have similar band structure. Except FeTi, the band structure of CoTi and NiTi are slightly shifted just below the Fermi level. The presence of bands at the Fermi level confirms that all the compounds are metallic in nature.

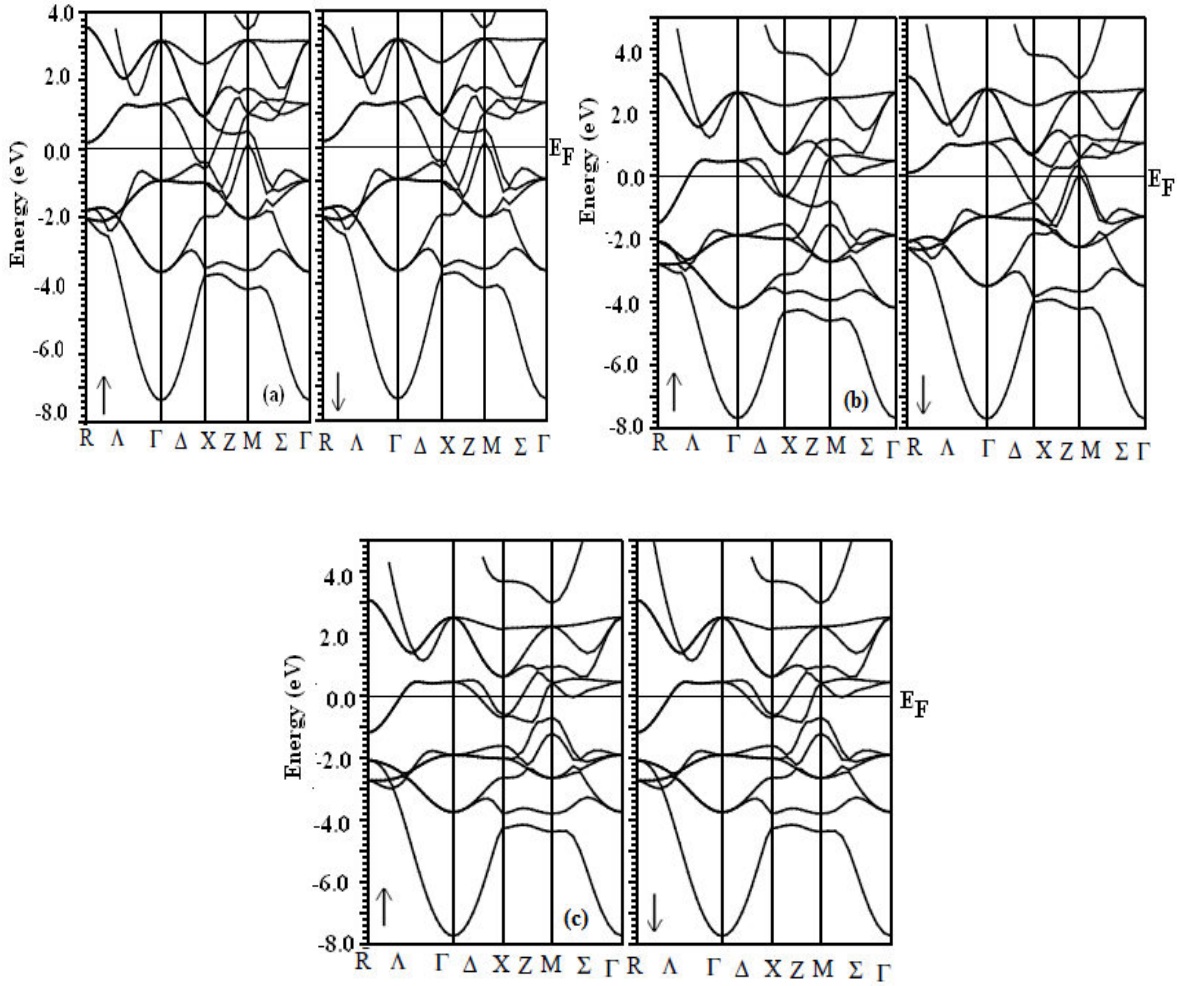

Figure. 2 Band structures for FeTi (a), CoTi (b) and NiTi (c)

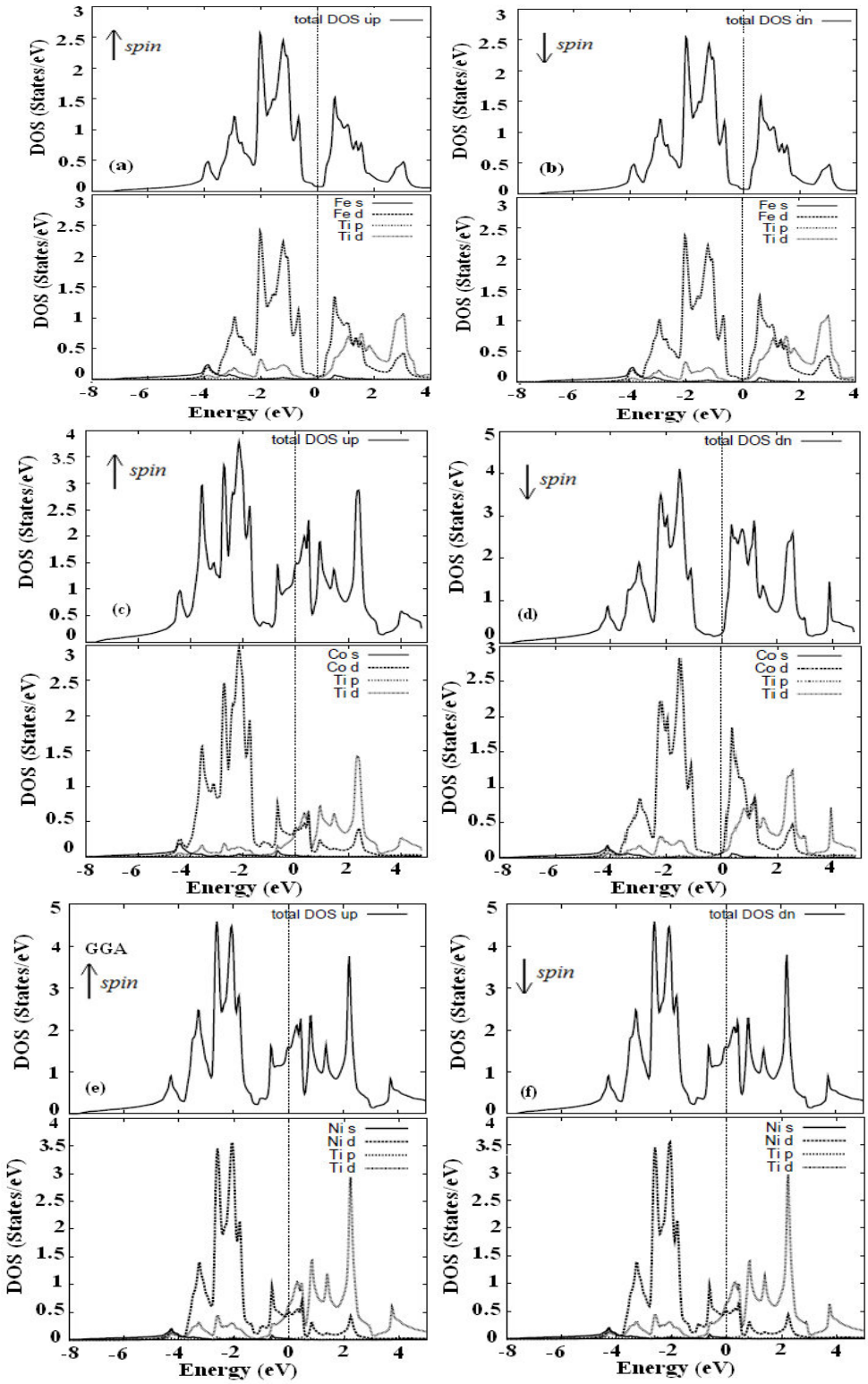

Figure. 3 Total and Partial DOS for FeTi (a, b), CoTi (c, d) and NiTi (e, f)

3.3 Elastic Properties

The elastic constants are important parameters that describe the response to an applied macroscopic stress and especially important as they are related to various solid state phenomena, such as bonding characteristic between adjacent atomic planes, anisotropic factor of binding and structural stability. We have calculated elastic constants of FeTi, CoTi and NiTi in B_2 phase at ambient pressure by using the method developed by Charpin and

integrated it in the WIEN2k package [18]. The calculated values of elastic constants are given in Table. 2 along with the available theoretical and experimental results. It can be noted that our calculated elastic constants satisfy the stability criterion: $C_{11} > C_{12}$, $C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} > B > C_{12}$ which clearly indicate the stability of these compounds in B_2 phase. Elastic constants play an important role for the determination of the mechanical properties as discussed in the next section.

Table 2. Calculated elastic constant and Young's modulus E, shear modulus G_H, anisotropic factor A, Poisson's ratio σ, B/G_H ratio and Cauchy's pressure C_{12}–C_{44} for MTi (M = Fe, Co and Ni)

Solids	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	E (GPa)	G_H (GPa)	A	σ	C_{12}–C_{44}	B/G_H
FeTi(GGA)	372.95	87.10	68.63	237.36	92.49	0.48	0.28	18.47	1.97
LSDA	445.28	130.28	109.80	322.76	126.95	0.69	0.27	20.20	1.85
Theo.	304[a]	139[a]	138[a]	283.58	13.08[a]	1.64[a]	0.25	-2	1.69
	385[c]	89.92[c]	81.13[c]	262.3[c]	103.4[c]	0.54	0.26	8.79	1.82[c]
CoTi(GGA)	286.51	113.79	74.66	205.74	79.13	0.86	0.29	39.13	2.16
LSDA	210.75	165.97	80.97	133.69	48.55	3.61	0.37	85	3.72
Expt.	203[a]	129[a]	68[a]	143.24	53.26[a]	1.83[a]	0.34	61	2.88
Theo.	261[a]	176[a]	99[a]	189.72	70.51[a]	2.32[a]	0.34	77	2.89
NiTi(GGA)	195.93	157.59	62.90	109.09	39.14	3.28	0.39	94.68	4.35
LSDA	218.38	184.32	54.92	97.51	34.41	3.22	0.41	129.40	5.68
Exp.	162[a]	132[a]	36[a]	71.74	25.33[a]	2.40[a]	0.41	96	5.60
Theo.	218[a]	178[a]	71[a]	119.68	42.87[a]	3.55[a]	0.39	107	4.46

[a]:Ref[12] [c]:Ref[17] Some parameters are derived from experimental and theoretical values of elastic constants.

3.4 Mechanical Properties

Elastic properties can be used to determine mechanical properties such as Young's modulus (E), shear modulus (G_H), Poisson's ratio (σ) and anisotropic ratio (A) for useful applications. We have calculated these properties of FeTi, CoTi and NiTi and presented them in Table 2. Using mechanical properties of these compounds based on their elastic properties, we have analyzed their ductility using the (B/G_H) ratio.

The shear modulus (G_H) describes the material's response to shearing strain using the Voigt-Reuss-Hill (VRH) method [24-26]. The Hill shear modulus (G_H) is given as:

$$G_H = \frac{G_V + G_R}{2} \quad (12)$$

Where $G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$ is the Voigt shear modulus (13)

and $G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$ is the Reuss shear modulus (14)

The Young's modulus (E) is important for technological and engineering application. Young's modulus is defined as the ratio of stress to strain, and is used to provide a measure of the stiffness of the solid, i.e., the larger value of E, the stiffer is the material. It is reported in the literature that stiffer solids have covalent bonds [27]. Young's Modulus (E) is given by-

$$E = \frac{9BG_H}{3B + G_H} \quad (15)$$

It can be seen from the Table 2 that the highest value of E occurs for FeTi implying stiffer material in nature as compared to CoTi and NiTi compounds. Another important parameter is the elastic anisotropic factor (A), which gives a measure of the anisotropy of the elastic wave velocity in a crystal and it is given as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (16)$$

which is unity for an isotropic material, anisotropy factor A is listed in Table 2.

The Poisson's ratio (σ) is given by eq (17) as

$$\sigma = \frac{3B - 2G_H}{2(3B + G_H)} \quad (17)$$

Using the mechanical and physical properties of these compounds based on their elastic properties, we have analyzed their ductility using the (B/G_H) ratio. The shear modulus (G_H) [24-26] represents the resistance to plastic deformation while the bulk modulus (B) represents the resistance to fracture. As suggested by Pugh [28], if $B/G_H < 1.75$; a material behaves in a brittle manner. Ganeshan *et al.* [29] have established a correlation

between the bonding and brittleness/ductility properties. The bond character of cubic compounds is explained with respect to their Cauchy pressure (C_{12} - C_{44}). Compound having more positive Cauchy's pressure tends to form bonds which are primarily metallic in nature, where as the compounds having more negative Cauchy's pressure from bonds which are more angular or covalent in character [30]. Thus the ductile nature of all MTi (M = Fe, Co and Ni) can be correlated to their positive cauchy's pressure and thereby metallic character in their bonds.

3.5 Thermal properties

With the help of calculated the Young's modulus (E), Bulk modulus (B_0) and the shear modulus (G_H), we have obtained the Debye temperature (θ_D) by using the average sound velocity v_m. At low temperature the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperature the Debye temperature calculated from elastic constants. We have calculated the average sound velocities (v_m) and Debye temperatures (θ_D) as well as the densities for B_2 phase by using the calculated elastic constants which are given in Table 3. In the absence of any measured data in the literature, they could not be compared. Hence, our results can be considered as a prediction for these properties of intermetallic compounds and it will testify future experimental work.

Table 3. Calculated longitudinal v_l, transverse v_t, average elastic wave velocities v_m, Debye Temperature θ_D for MTi (M = Fe, Co and Ni)

Solids	$\rho*10^3$ (kg/m^3)	v_l (ms^{-1})	v_t (ms^{-1})	v_m (ms^{-1})	θ_D (K)
FeTi (GGA)	5.064	7867	4406	4900	352.20
LSDA	5.413	8670	4880	5425	398.66
Other Theo.	5.539	7916	4583	5083	376.43
Other Theo.	5.091	7989	4551	5054	366.63
CoTi (GGA)	5.091	7377	3947	4405	314.08
LSDA	5.530	6825	3225	3626	265.78
Expt.	5.098	6684	3302	3704	264.21
Other Theo.	5.149	7711	3851	4317	308.99
NiTi (GGA)	4.955	6826	3026	3413	241.35
LSDA	5.345	6821	2727	3087	223.86
Expt.	4.985	5988	2352	2664	188.78
Other Theo.	5.350	6954	3075	3468	251.57

These values are derived from experimental and theoretical values of elastic constants.

4. Conclusion

First principles calculation have been performed on MTi (M = Fe, Co and Ni) intermetallic compounds by FP-LAPW method using DFT with both GGA and LSDA. Our results on the structural, electronic, elastic, mechanical and thermal properties are in good agreement with other experimental and available other theoretical results. The calculated elastic constants show that FeTi, CoTi and NiTi are elastically stable in B_2 phase. Using these elastic constants the shear modulus (G_H) , poisson's ratio (σ), young's modulus (E) and anisotropy factor (A) are also reported. The electronic band structures show the metallic character for all compounds. In the present study we found B/G_H ratio > 1.75 and C_{12}-C_{44} > 0 which implies that all these compounds are ductile in nature and NiTi have an excellent ductility amongst all the compounds. We have also analyzed that the more delocalized bands are present in NiTi at Fermi level (E_F) as compared to FeTi and CoTi. The thermal properties are also reported for these compounds.

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