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Regular Article

Insight into the physical properties of the inter-metallic titanium-based binary compounds

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Abstract Herein, we present the structural, magnetic, electronic along with elastic properties of inter-metallic X_3Ti (X = Ce, Eu, Nd, Pm and Yb) compounds studied using density functional theory (DFT). These features are computed by means of the full potential linearized augmented plane wave (FP-LAPW) process within the generalized gradient of exchange and correlation approximation with the added Hubbard U-term for on-site coulomb interaction (GGA + U). The ground state properties including the lattice parameter (a_0), the bulk modulus (B) and its pressure derivative (B′) are computed which are consistent with the experimental along with other theoretical findings available. The metallic behavior of all these compounds is revealed by the band structures. Sub-orbitals of the transition/lanthanide elements comprising d and f have a massive significance to those of the density of states. We have investigated also the magnetic properties of X_3Ti (X = Ce, Eu, Nd, Pm and Yb) inter-metallic compounds using a GGA + U. By calculating the magnetic moments for all the investigated compounds, we found that all our compounds represent ferromagnetic behavior. We have computed the elastic constants for these compounds for the first time. Elastic parameters indicate value for shear modulus (G), bulk modulus (B), Young's modulus (Y), Poison's ratio (v) and anisotropy (A) which eventual results in ductility, strength, toughness and brittleness of these materials in accordance with Pugh's criteria. With the accord of Pugh's criteria, we have reported that all our compounds are brittle. The above findings may add comprehensive insight in understanding the physical properties of Ti-based intermetallics.

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1 Introduction

Rare earth intermetallics have been considered as attractive materials due to their large technological applications, especially in permanent magnets as well as because of their outstanding structural, mechanical, stability at high temperatures, mechanical and chemical properties [1, 2]. These compounds with crystal structure like $AuCu_3$ and remarkable magnetic properties have deserved intensive investigations for the promising industrial applications. Klasse et al. [3] have investigated some of the Yb-based compounds for their anomalous magnetic behavior. In $YbIn_3$, complicated meta-magnetism of numerous anti-ferromagnet and di-valency has been studied [4]. By ab-initio method, in rare earths RIn_3 and RSn_3, the valency and the electric field gradients have been studied [5]. For RSn_3 (R = Sm, Eu, Gd) and RIn_3 (R = Tm, Yb, Lu) compounds, the influence of spin polarization on structural properties and electric field gradients has also been explored. For rare earth intermetallic compounds, for instance, GdM (M = Cu, Ag, Mg) and RIn_3 (R = Gd, Tb, Dy), the effect of pressure on the magnetic susceptibility has been investigated [6]. Similarly, Abraham et al. studied the structural, mechanical, electronic and elastic properties of $REIn_3$ and $RETi_3$ intermetallic compounds via ab-initio calculations [7]. Influence of high pressure on the structural properties of lanthanide trialuminides has been examined by Vucht and Buschow [8]. Amin et al. [9] investigated binary intermetallic compounds XAl_3 via first principle calculations. However, there exists very rare literature on X_3Ti compounds, which ignited us to carry out the present work. Therefore, in this work, we compute to investigate the structural, electronic, magnetic and elastic properties of X_3Ti (X = Ce, Eu, Nd, Pm, Yb) within the approach of DFT.

2 Computational methodology

In this work, the calculations were carried out with full potential linearized augmented plane wave (FP-LAPW) method [10] build in the DFT as incorporated in the WIEN2K code [11]. To deal with the exchange correlation potential, the generalized gradient of exchange and correlation approximation with the added Hubbard U-term for on-site coulomb interaction (GGA + U) [12] is used, where the value of U is taken to be 0.52 (Ry). Structural parameters are obtained by using Murnaghan's state equation and fitting the energy versus volume curve [13]. The unit cell of crystal compound is divided in different domains within the full potential scheme: (1) atomic spheres and, (2) interstitial region (outside region of the atomic spheres). The wave function is split to two distinct basis sets and is extended in atomic like functions (radial function time's spherical harmonics) in each atomic sphere, while it is extended into a plane wave basis in the interstitial region. In expressions of spherical harmonics, the wave function is expanded to $l = 12$. Similarly, the potential is expended as

$$V(r) = \begin{cases} \sum\limits_{lm} V_{lm}(r) Y_{lm}\left(\hat{r}\right) \\ \sum\limits_{K} V_K \mathrm{e}^{iKr} \end{cases} \tag{1}$$

Inside of the sphere is represented by Eq. (1) is for the interstitial domain. For this study, the muffin-tin sphere radii RMT values are chosen in such a manner that charge is isolated in the core hence no leakage of charge ensuring the total energy. RMT values for Ce, Eu, Nd, Pm and Yb is 2.5, for Ti is 2.5. The cutoff parameter RMT $\times$ K_{max} is taken 7. K points have been taken as 1000 to acquire satisfactory and reliable findings. For the magnetic properties of these X_3Ti intermetallic compounds, calculations with spin polarized within GGA + U is employed. The spin magnetic moments are calculated for the total, interstitial and electronic

part. The DFT method has proven to be one of the most accurate methods for the computation of the electronic structure of solids [14–16].

3 Results and discussion

3.1 Structural properties

Rare earth intermetallic compounds of A_3B type having two atoms in the crystalline structure with a Pm-3 m (No 221) space group, in which rare metals are at the corner position of the unit cell and transition metal Ti at the face-centered, shown in Fig. 1

The measurement of ground-state structural parameters were found out through Burch Murnaghan equation of state in which total energy versus volume are fitted, consequently bringing the system to optimized state [13]. Figure 2 depicts the fitted Murnaghan curve, by which the structural parameters like ground state energy, bulk modulus, lattice constant, derivative of bulk modulus, ground state volume are computed and are presented in Table 1. Equilibrium state of the system can be estimated from the point in the fitted curve having the lowest energy corresponding to that volume and the parameters like energy and volume relative to that point is considered to be energy at ground state with volume at ground state or optimum volume. And these parameters can be further used for the computation of other lattice parameters at the ground state.

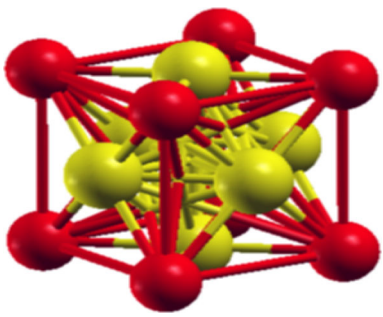

Fig. 1 Schematic prototype crystal structure of X_3Ti, the red color and yellow colors depict Ti and X, atoms respectively

Table 1 Computed X_3Ti (X = Ce, Eu, Nd, Pm and Yb) structural parameters at the ground state

Compounds	a_0 (Lattice constantsin Å)	B_0 (Bulk Modulus in GPa)	$B^{/}$ (Pressure Derivative of B_0)	Volume in Ground state (V_0)	Energy in Ground State E_0 in Ry
Ce_3Ti	4.6099	51.3800	5.2429	661.5762	−54,899.782606
Eu_3Ti	5.0219	9.6555	−6.0460	854.6874	−66,822.344904
Nd_3Ti	4.7645	37.4237	8.9565	729.8878	−59,487.873763
Pm_3Ti	4.7715	43.7779	18.4390	733.1044	−61,871.531989
Yb_3Ti	4.8005	27.8623	4.7499	746.5638	−86,162.993228

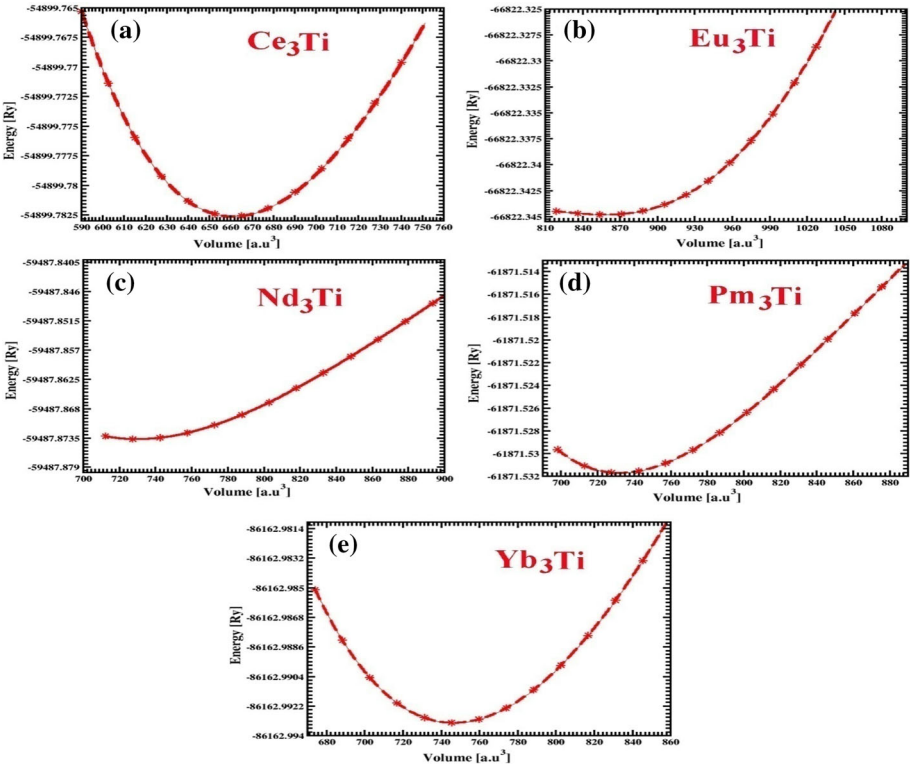

Fig. 2 Structural optimized curve in response to unit cell volume of X_3Ti

3.2 Electronic properties

The X_3Ti intermetallic compounds electronic properties are examined at 0 K and 0GPa, for instance, band structures, total and partial density of states (TDOS, PDOS) and electron density. Figure 3 illustrates the band structures of X_3Ti (X = Ce, Eu, Nd, Pm &Yb). It can be seen that the bands for all the investigated compounds overlap at Fermi level, i.e., no gap occur between the valence band and conduction band. This overlapping nature at the Fermi level shows that all of our compounds are metallic in nature with band gap of 0 eV.

Explaining further the electronic properties, band structures are explained from the DOS. The TDOS and PDOS for all the compounds are calculated for the configuration of both spin up and spin down as shown in Fig. 4. It can be observed from the figure that in both TDOS and PDOS spin up and down configuration, the major contribution is due to X atom, where X = Ce, Eu, Nd, Pm &Yb. And this major contribution of X atom is because of X-f atomic state. It can be also seen from the figure that the contribution to TDOS and PDOS is contributed from the transition Ti atom and both configuration of spin up and spin down. The configuration X atom ranges from −2.5 to 6.5 eV in spin up case as well as in spin down case.

The nature of chemical bonding is explained from the electron charge density. The electronic charge densities along (100) plane for all the binary intermetallic compounds are shown in Fig. 5. It can be seen that the shape of X (X = Ce, Eu, Nd, Pm &Yb) atom is completely

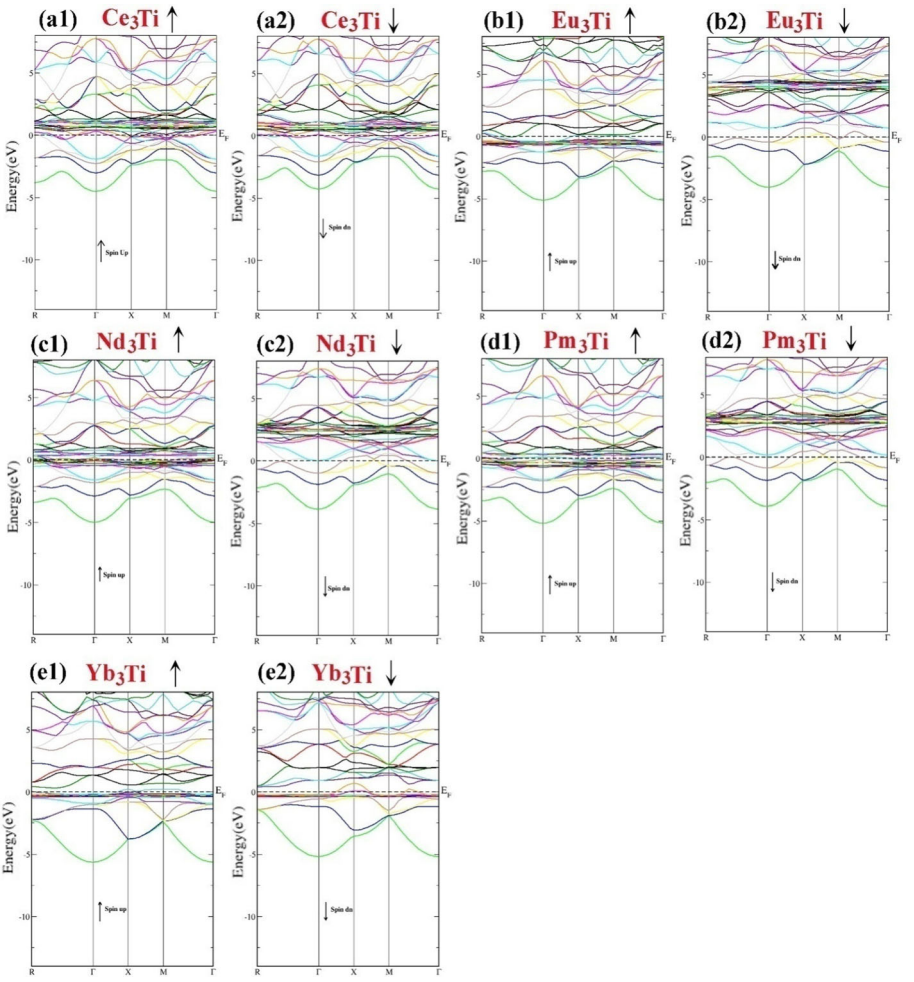

Fig. 3 Band structure of X_3Ti (X = Ce, Eu, Nd, Pm &Yb)

spherical inside the sphere, which shows that the f-state of X is completely filled. Also Ti atoms show completely spherical shape and represents that the d-state of atom Ti is filled. Thus, the bonding between X-Ti is totally ionic.

3.3 Magnetic properties

In order to find out the magnetic properties of the rare earth binary intermetallic X_3Ti compounds are calculated by applying spin polarized calculations within the GGA + U approximation. The computed magnetic moments and total, interstitial and local are shown in Table 2.

The major contribution to the magnetic moments of the under study compounds is due to the transition element, i.e., lanthanide series comprising Ce, Eu, Nd, Pm and Yb. The contribution of lanthanide series to the total magnetic moment is 1.45128 μ_B, 6.50872 μ_B, 3.48289 μ_B, 4.55985 μ_B and 1.52180 μ_B, whereas the contribution of transition element to the

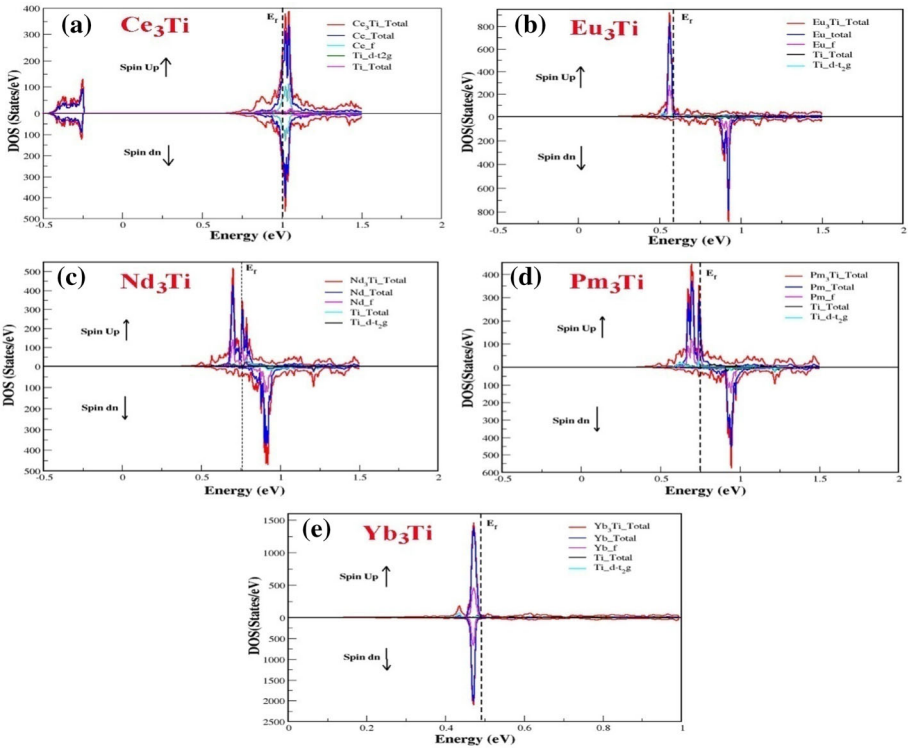

Fig. 4 Total and partial density of states (TDOS, PDOS) for X_3Ti (X = Ce, Eu, Nd, Pm &Yb) for both spin up and spin down configuration

total magnetic moment is 1.78783μ_B, 1.74220 μ_B, 1.75465 μ_B, 1.71637 μ_B and 1.76845 μ_B, respectively. It is also found that the DOS of X_3Ti in both spin up and spin down cases follow the similar trend, indicating that there is a ferromagnetic nature for all the compounds, shown in Fig. 4. From Table 2 it can be seen that there is a little contribution of the interstitial atoms to the total magnetic moments of 1.78501 μ_B to Ce_3Ti, 1.74236 μ_B to Eu_3Ti, 1.83103 μ_B to Nd_3Ti, 1.78539 μ_B to Pm_3Ti and 1.61288 μ_B to Yb_3Ti. Among these studied compounds, Eu_3Ti exhibits the strong ferromagnetic behavior as the value of total magnetic moment is 24.01073 μ_B. Similar studies has been carried out investigating the magnetic behavior of intermetallic compounds by Murtaza et al. [17] exhibiting ferromagnetic behavior for some of the compounds.

3.4 Elastic properties

We have determined the elastic constants (C_{11}, C_{12} and C_{44}), for account the intermetallic compounds X_3Ti (X = Ce, Eu, Nd, Pm &Yb) and correlated them with the forthcoming results. Table 3 display all computed elastic constant for all compounds under investigation. The $C_{11} + 2C_{12} > 0$, C_{11}—$C_{12} > 0$, $C_{44} > 0.4$, $B > 0$ is criteria for the mechanical stability of the cubic compounds [18, 19]. From such elastic constants, the mechanical properties of such substances, comprising bulk modulus (B), Young's modulus (Y), anisotropy (A), shear modulus (G) and Poison's ratio (v) for all materials are investigated. The toughness of the

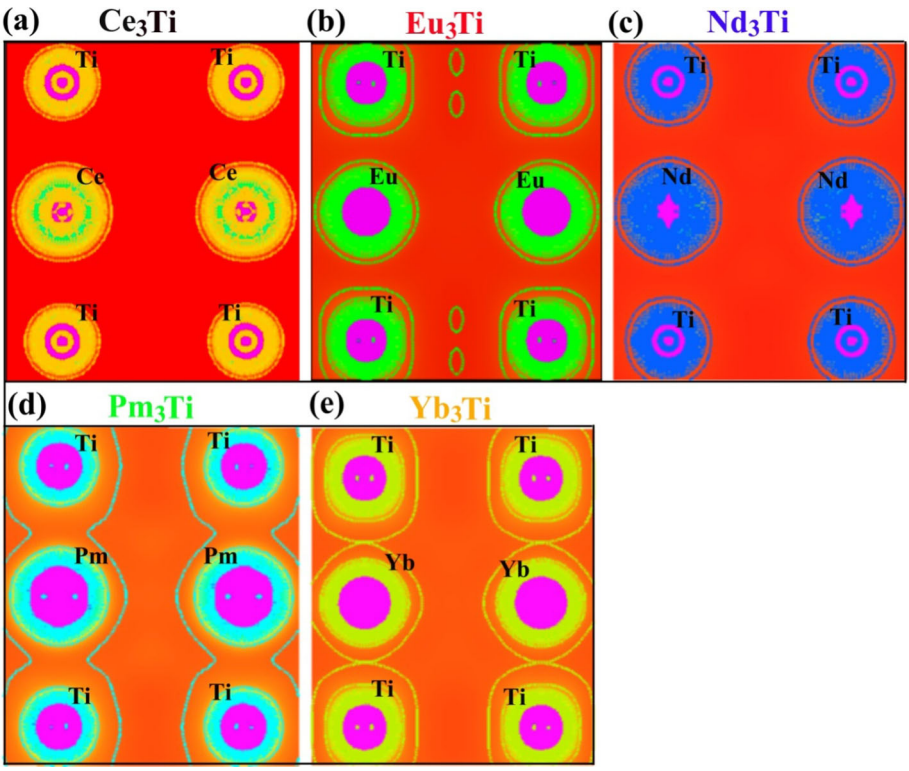

Fig. 5 Electronic charge density of X_3Ti (X = Ce, Eu, Nd, Pm &Yb)

Table 2 Computed total (m^{tot}), interstitial (m^{int}) and local (m^{*1}, m^{*2}) magnetic moments with GGA potential

S. no	Compounds	m^{int}	m^{*1}	m^{*2}	m^{tot}
1	Ce_3Ti	1.78501	1.45128	1.78783	7.92669
2	Eu_3Ti	1.74236	6.50872	1.74220	24.01073
3	Nd_3Ti	1.83103	3.48289	1.75465	14.03435
4	Pm_3Ti	1.78539	4.55985	1.71637	17.18130
5	Yb_3Ti	1.61288	1.52180	1.76845	7.94674

compound can be indicated from the shear modulus (G). For all compounds, the computed values of the shear moduli under analysis are shown in Table 3. From the table, it is visible that Eu_3Ti has 104.356 Gpa, which is the highest shear modulus value among all compounds, which indicates that Eu_3Ti is the hardest of all of these compounds.

Is from above table it is clearly depicted that −149.344 Gpa is smallest value of shear modulus for Ce_3Ti, which correspond a very small opposition for deformation existed for this compound. The stiffness of a material can be displayed from Young's module E [20]. Table 3 demonstrates the investigated value for all inter-metallic binary X_3Ti compounds. It very clear that Nd_3Ti possess 50.185 Gpa numerical quantity of E, which indicate the high material stiffness in comparison to others. Higher values of Young's modulus comparative to the shear modulus indicate the stiffness of these materials. From an engineering perspective, the B/G is significant ratio of the material for ductility. The B/G threshold value for material

Table 3 Calculated elastic parameters C_{11} (in GPa), C_{12}(in GPa), C_{44}(in GPa), B (in GPa) A, G (in GPA), E(in GPA), υ, B/G, B/C_{44})

S. no	Compound	C_{11}	C_{12}	C_{44}	B	A	G	E	υ	B/G	B/C_{44}
01	Ce_3Ti	31.85	16.68	52.006	21.30	6.309	104.3	5.582	−1.18	0.204	0.4096
02	Eu_3Ti	42.45	57.86	−462.5	52.55	62.18	−149.3	−8500	−5.15	−0.352	−0.1136
03	Nd_3Ti	17.70	13.90	29.18	14.31	9.142	12.82	29.61	0.209	1.116	0.490
04	Pm_3Ti	−15.91	38.98	−82.32	20.05	3.106	−52.34	−1207	−6.74	−0.383	0.243
05	Yb_3Ti	43.13	18.37	30.003	26.47	2.379	21.19	50.18	0.250	1.249	0.882

to be ductile is larger than 1.75, and if a material possess lower than 1.75, it is said to be brittle material behavior [21]. The B/G ratio measured for all X_3Ti (X = Ce, Eu, Nd, Pm &Yb) is shown in Fig. 3. Table express the B/G ratio for all the materials, and its value is less than the threshold 1.75, consequently all of our analyzed compounds are brittle in nature. The material ductility/brittleness nature can also be characterized by a parameter known as Cauchy's pressure of the form ($C'' = C_{12} - C_{44}$). The positive and negative values of Cauchy's pressure represents the ductility and brittleness nature, respectively [18]. Another parameter seems to be very significant is the ratio of Poisson that can be used to state the various mechanical properties, i.e., the incompressibility. The critical numerical quantity of Poisson ratio lies in between 0 and 0.5 and improves incompressibility occurrence when varying from 0 to 0.5 [22]. The values of Poisson ratio computed for all the materials are displayed in Table 3. It is noticeable from the table that Nd_3Ti and Yb_3Ti has 0.209 and 0.250 ratios of Poisson, respectively, which fall within in the above limit; thus in resultant, these compounds against deformation are low compressible. Moreover, to evaluate the existence of the inter-atomic forces, this ratio is often used. The standard range of the ratio of Poisson to the central forces is 0.25 and 0.5 [23]. The approximated values of the Poisson ratio show that the prevailing inter-atomic forces Nd_3Ti and Yb_3Ti compounds are the central forces, while for the rest of the compounds, the forces are non-central. A parameter which shows that whether or not a material structural properties stay identical in all direction is an anisotropy factor (A). For A = 1, the medium is isotropic and if A deviates from 1, the medium is anisotropic. The anisotropic ratios estimated for all compounds are shown in Table 3. The table list presents that for all these compounds, the anisotropic ratio deviates from 1, which express that their properties vary in various directions. Thus, all these compounds are anisotropic. B/C_{44} which is the ratio of bulk modulus to C_{44} may be used to investigate a material plasticity [24]. Table 3 shows the B/C_{44} for such compounds. From the table, it is detectable that the ratio B/C_{44} is larger for Yb_3Ti (0.882 GPa) and the lower for Ce_3Ti. This higher B/C_{44} value for Yb_3Ti imply a high degree of plasticity as compared to else.

4 Conclusion

Structural, magnetic, electronic and elastic properties of binary rare earth intermetallic compounds X_3Ti (X = Ce, Eu, Nd, Pm &Yb) have been computed with FP-LAPW process with the GGA + U approximation in wien2k simulation code. The calculated structural parameters including the lattice parameter (a_0), the bulk modulus (B) and its pressure derivative (B′) are found to be in good agreement with the available literature. The significant contribution to the DOS resulted from sub-orbitals d & f of transition lanthanide series elements comprising Ce, Eu, Nd, Pm and Yb. The nature of chemical bonding is explained from the electron charge density, which shows that the bonding between X-Ti is totally ionic. Magnetic properties of the rare earth binary intermetallic X_3Ti compounds are calculated by applying spin polarized calculations within the GGA + U approximation. From the calculation of magnetic moments, it is resulted that our compounds are ferromagnetic in nature. Elastic parameters indicate value for bulk modulus (B), Young's modulus (Y), shear modulus (G), anisotropy (A) and Poison's ratio (v), which results in ductility, strength, toughness and brittleness of these materials in accordance with Pugh's criteria. It is concluded that all our materials are brittle in nature. We are fully confident on the accuracy of our reported properties for X_3Ti and can be deemed its applications in high-performance electronic and magnetic devices.

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