Physics of semiconductor devices & renewable energies journal

Vol. 01 n. 01 (2023) ; ISSN 2992-040X
Journal homepage: www.psdrej.com

Contribution to the study of the CoFeTi Asquaternary Heusler material's structural, electronic, and magnetic properties

Fatima SOFRANI[1]*, Keltouma BOUDIA [2] and Friha KHELFAOUI[2,3]

[1] *Département des Science de la Matière , Faculté des Sciences et de la Technologie, Universitaire El Wansharissi Tissemsilt ,*
[2] *Laboratory of Physico-chemistry of Advanced Materials, University of Djillali Liabes, BP 89, Sidi-Bel-Abbes 22000, Algeria,*
[3] *Laboratoy of physico-chemical studies University of Saida Dr Moulay Tahar, Saida, Algeria*
*Corresponding author *Email: fatima.sofrani@cuniv-tissemsilt.dz*

Abstract

By simulating the structural, electronic, and magnetic properties of the QuateryCoFeTiAs Heusler compound, we presented a theoretical investigation in this work The calculations were performed using the generalized gradient (GGA) approximation and the WIEN2k code's application of the augmented plane wave method (FP-LAPW)which is based on density functional formalism (DFT). The results are consistent with important theoretical calculations**.**Our results showed that this compound conforms with the (Slater-Pauling) Mtot = (ZT - 24) μ_B rule and is a half-metallic material**.**

Keywords: *magnetic properties 1 ;DFT 2; Slater-Pauling 3 ; half-metallic 4*

1. Introduction

The discovery of the Heusler 1903 compounds attracted increasing interest because of their interesting properties in practical applications such as magneto-electronics and spintronics [1.2]. They remain attractive for other technical applications like spin injection devices, tunnel junctions or devices due to their high Curie temperature compared to these compounds [3]. Heusler compounds are intermetallic compounds usually consisting of two transition metals (X or X', Y) and a main group element (Z). They can be divided into three groups: Compounds with the chemical formula XX'YZ have four fcc subarrays and others with the formula X2YZ [4]. Ozdogan et al studied 60 quaternary Heusler alloys, where all compounds obey the Slater-Pauling rule in which 41 compounds are half-metals, 8 compounds are spin-gapless semiconductors, 2 compounds are magnetic semiconductors, and 9 are semi-conductors [5]. The main objective of the research work carried out in this paper is the ab initio study of the structural, electronic, and magnetic properties of the Heusler CoFeTiAs quaternary alloy using the method of linearized augmented plane waves at total potential (FP-LAPW). Using the generalized gradient approximation PBE–GGA, implemented in the Wien2k code.

2. Materials and Methods

The studies in this section's results were performed using the WIEN2k code and the Density Functional Theory (DFT). The Full Potential Linearized Augmented Plane Wave (FP-LAPW) method is implemented in this code [6.7.8]. The generalized gradient approximation (GGA) of Perdew, Burk, and Ernzerhof provides a description of the exchange and correlation energy.[9.10] Combining spherical harmonics in the atomic spheres, or surrounding the atomic

sites, with the Fourier series in the interstitial areas allows for the development of the fundamental functions, electronic densities, and potentials. The parameter RMT*Kmax is set to 8, where Kmax is the greatest reciprocal vector modulus in the first Brillouin zone and RMT is the lowest muffin-tin radius of the sphere MT during the calculations by the WIEN2k code. The integration of the Brillouin zone is carried out with 3000 k-points.

3. Results and discussions

3.1. Structural properties

In a first-principles calculation, the most important step is to determine the structural properties of a given system in its ground state. The Heusler quaternary CoFeTiAs alloy can have three different types of structures as shown in the figure.1 and Table1.

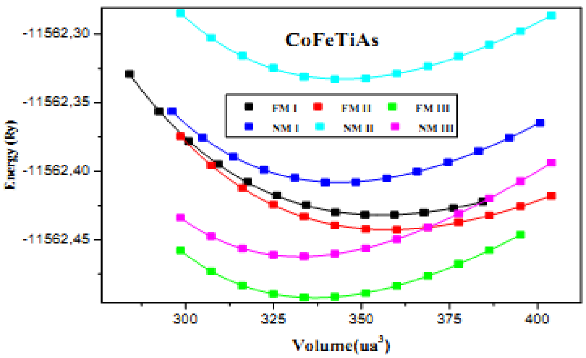


Figure1. Optimization of total energy as a function of volume using the GGA approximation.

Table 1. The different types of structure for the compound CoFeTiAs.

	(0, 0,0)	(1/4,1/4,1/4)	(3/4,1/4,1/4)	(1/2.0.0)
Type I	Co	Fe	Ti	As
Type II	Co	As	Fe	Ti
Type III	Co	Ti	As	Fe

3.1.1 Total energy and lattice parameters

The structure of the quaternary alloy was optimized by calculating the total energy as a function of volume and then fitting the data to the Birch-Murnaghan equation of state. In order to obtain the ground state structure of our alloy and the favorable magnetic state, we performed total energy versus volume calculations for the three different types of structures possible for the non-magnetic (NM)
and ferromagnetic (FM) phases. equation of state[11]:

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B' + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \quad (1)$$

From Fig(1). We observe that Our Compound is more stable in the type III ferromagnetic phase because the corresponding energy is the lowest. The settings are as follows: volume V_0, compressibility modulus B and its first derivative B' which corresponds to the equilibrium state are calculated using the approach GGA.and they are grouped in the following table:

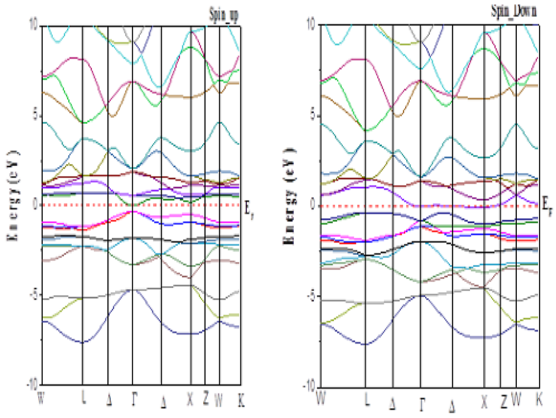
Table 2. Lattice parameter a (A°), lattice volume, modulus of compressibility B (GPa), its derivative B' and the total energy (eV) of the CoFeTiAs allye.

Les types alliage CoFeTiAs	a(A°)	V_0	B(GPa)	B'	E_0
FM-I	5.8495	355.6636	139.5955	4.4370	-11562.4318
FM- II	5.8535	357.5238	149.9660	4.3122	-11562.4426
FM- III	5.737- 5.71 [12]	336.8043	184.5370	4.9633	-11562.4922
NM- I	5.7991	343.6202	177.6876	4.3831	-11562.4080
NM- II	5.7971	344.5441	177.7184	4.4644	-11562.3327
NM- III	5.7240	332.4630	194.0557	5.0829	-11562.4622

3.2. Electronic properties

3.2.1 Band structure

We studied the electronic band structure of the quaternary Heusler alloy, where we will use the equilibrium lattice parameter corresponding to the phase FM. The band structure represents the reciprocal space subject to the dispersion relation, which helps us better understand the phenomenon of half-metallicity in an alloy. Fig 2 (a.b) shows the band structures of the alloy studied at points and along the high symmetry directions of the first Brillouin zone for the two cases of spin-up and spindown, respectively. From Figure 2 (a), we see a Fermi level (EF) interference for the majority of spins, which shows semiconductor behavior where the valence band maximum and conduction band minimum coincide at the same point of symmetry, meaning that 'it has a direct gap around the Fermi level of value Eg= 0.327 eV. On the other hand, from Fig 2(b), the compound has a metallic character (i.e. the gap is zero) in the direction of the minority spins.



(a) (b)

Figure 2: Electronic band structure of the majority and minority spins of the quaternary Heusler alloy CoFeTiAs.

3.2.1.Density of electronic states

The density of states is generally used to understand the electronic structure of a compound in detail. The total and partial state densities of the CoFeTiAs alloy in the ferromagnetic phase are computed in their stable state using the GGA approximation, and they are shown in Fig(3) as a result.

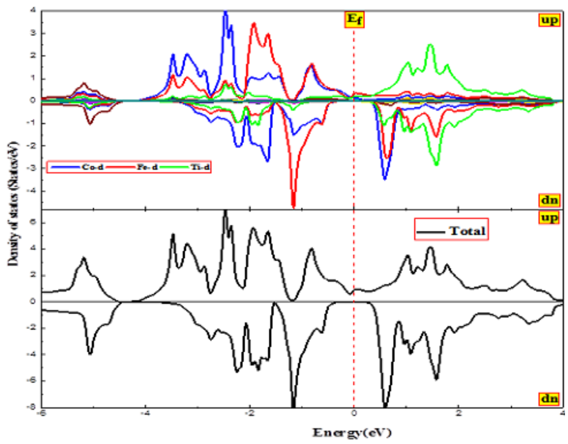


Figure 3. Total and partial state densities of the majority and minority spins of the quaternary Heusler alloy CoFeTiAs with the equilibrium lattice parameter.

Fig(3) shows the electronic states of Fe, Co, and Co atoms at the Fermi level. The graphs confirm a strong hybridization of the d-Fe and d-Co orbitals described above, in the energy range between -2 and 2 eV. It is clear that the majority electrons (spin-up) have a semiconductor character, while minority spins have a metallic behavior, confirming the property of half-metallicity. For our compound, the total density of states is mainly dominated by the d states of the Co, Fe, and Ti atoms. For the atom. We see that these states' contribution is Negligible for the p state of the As atom in the energy range from – 6.6 eV to – 2.5 eV.

3.3. Magnetic properties

Using the GGA approximation, the total M_{TOT}, interstitial Mint, and atomic magnetic moments of the quaternary Heusler compound CoFeTiAs were calculated. The results are summarized in table .3.

Table 3. Total and partial magnetic moments in (μ_B) and spin polarization for the quaternary Heusler compound CoFeTiAs.

	MCo	MFe	MTi	MAs	Mint	MTot	Px100
CoFeTiAs	1.083	1.144	-0.151	0.038	-0.097	2.000	100%

The magnetic moment of our compound is 1 μ_B, satisfying SlaterPauling's rule[13]:

$$M_t = Z_t - 24 \quad (2)$$

Z_t: is the total number of valence electrons:

Z_t = 26

M_t = 26 - 24 = 2 μ_B

This compound is a half-metallic material and obeys the (Slater–Pauling) rule. The contribution of each atom gives us the magnetic phenomenon. We observe that the contribution of the elements Fe, of Co is very important, and that the two elements Ti and Si, have negligible magnetic moments.The magnetic moment of this compound is due to the strong contribution of the 3d-Fe states around the fermi level EF.

In the absence of results for this compound, we can only speculate as to how strong the magnetic field may be in this compound.

4. Conclusion

This paper contributes to explaining the current status of calculations in density functional theory and this by the linearized plane wave method (FP-LAPW) implemented in the Wien2K code. Ab-initio type simulations could come complement or even replace experimental data. Theoretical calculations are able to support the experiment by confirming hypotheses or by providing a fundamental interpretation of a concrete phenomenon. allowed us to better learn the structural, electronic, and magnetic aspects of the CoFeTiAs material belonging to the family of quaternary Heusler alloys. for Structural properties They have found that it is stable for (FM) con-figuration in structure type III and that it's The alloy CoFeTiAs has a direct gap in the majority spin and magnetic interactions are ferrimagnetic between Co and Fe, and between Fe and Co. All these properties make it possible to say that the alloy has one character, that is, it is half metallic. The spin polarization is 100% in addition to the Slater-Pauling rule Mt=26-24=2 u_B and the magnetic properties of each atom as well as the total magnetic moment are verified. According to the results obtained we can classify this material as an inciting candidate for spintronic applications.

References

1. Hu, R., Z. Fan, "Structural stability, magneto-electronics and spin transport properties of triangular graphene nanoflake chains with edge oxidation." Carbon 126: 93-104. et al. (2018).
2. De Groot, R., F. Mueller, "New class of materials: half-metallic ferromagnets." Physical Review Letters 50(25): 2024. et al. (1983).
3. Felser, C. and G. H. Fecher Spintronics: from materials to devices, Springer Science & Business Media.et al(2013).
4. Gao, Q., I. Opahle, "High-throughput screening for spin-gapless semiconductors in quaternary Heusler compounds." Physical Review Materials 3(2): 024410. et al. (2019).
5. Skaftouros, S. and K. Özdogan "E. S-as-ıoglu and I. Galanakis." Phys. Rev. B: Condens. Matter Mater. Phys 87: 024420.et al(2013).
6. Blaha, P., K. Schwarz, "wien2k." An augmented plane wave+ local orbitals program for calculating crystal properties 60. et al. (2001).
7. Berri, S., D. Maouche"A first-principle study of half-metallic ferrimagnetism in the CoFeTiSb quaternary Heusler compound." Journal of magnetism and magnetic materials 354: 65-69. , et al. (2014).
8. Halder, M., M. Mukadam, "Electronic, structural, and magnetic properties of the quaternary Heusler alloy NiCoMnZ (Z= Al, Ge, and Sn)." Journal of Magnetism and Magnetic Materials 377: 220-225. et al. (2015).
9. Perdew, J., K. Burke, "Perdew, burke, and ernzerhof reply." Physical Review Letters 80(4): 891. et al. (1998).
10. Zhao, Y., N. E. Schultz, "Exchange-correlation functional with broad accuracy for metallic and nonmetallic compounds, kinetics, and noncovalent interactions." The Journal of chemical physics 123(16): 161103. et al. (2005).
11. Wen, Z., Z. Zou, "First-principles study of phase stability, elastic and thermodynamic properties of AlCrFeNi medium-entropy alloys." International Journal of Modern Physics B 34(25): 2050218. et al. (2020).
12. Khenata, R., M. Sahnoun, "Full-potential calculations of structural, elastic and electronic properties of MgAl2O4 and ZnAl2O4 compounds." Physics Letters A 344(2-4): 271-279. et al. (2005).
13. Skaftouros, S., K. Özdoğan"Generalized Slater-Pauling rule for the inverse Heusler compounds." Physical Review B 87(2): 024420. , et al. (2013).