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DFT Studies on Structural Stability and Magnetic Properties of XTiSb (X=Fe,Co)

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Abstract: *The structural stability of titanium based magnetic materials XTiSb (X=Fe,Co) is investigated by calculating the total energies for both magnetic and nonmagnetic phases by the first principles calculations based on density functional theory using Vienna ab-initio simulation package (VASP). The ground state parameters such as lattice constant, cell volume and bulk modulus are calculated. The calculated lattice parameters are in agreement with earlier reported values. The mechanical parameters like elastic constants, bulk modulus, Youngs modulus, Poisson's ratio and B/G ratio are estimated. The calculated magnetic moments of FeTiSb and CoTiSb are 0.906 μ_B and 0.001 μ_B, which indicate that FeTiSb is stable in magnetic phase and CoTiSb is in nonmagnetic phase. The density of states reveals that FeTiSb is a half metallic with an energy gap of 0.576 eV and CoTiSb is a semiconductor with an energy gap of 1.013 eV at ambient condition.*

Keywords: *Ab-initio calculation, Electronic structure, Magnetic property, Mechanical properties.*

I. Introduction

Titanium and its alloys are attractive metallic materials which are widely used as implants for dental, restorations and orthodontic wires as well as orthopaedic due to their non-corrosive, low density and biocompatibility **[**1]. Titanium alloys have low modulus, good fatigue strength, formability, machinability, low thermal conductivity, high strength to weight ratio, than in many other structural materials, which have made them desirable for industry, medicine, dentistry and aeronautical applications [2]. Titanium based ternary intermetallic half heusler alloys XYZ crystallized in the cubic (CI_b) structure have attracted more attention because they posses wide variety of interesting physical properties such as very high seeback coefficient, electrical resistivity and thermal conductivity. In the present work, the structural, mechanical, electronic and magnetic properties of Titanium based Half Heusler magnetic materials FeTiSb and CoTiSb for possible nonmagnetic and magnetic phases are reported.

II. Computational Details

In this work, all the calculations are performed using the Vienna Ab-initio Simulation Package (VASP) code within the density functional theory frame work, where the PBE form of GGA [3,4] was employed to describe the electron exchange and correlation. The calculations are carried out with an energy cut-off 350eV for both the alloys and the Brillouin zone integration performed with a mesh of 4X4X4 generated by Monkhorst-pack method for both FeTiSb and CoTiSb alloys. The valance electronic configuration for FeTiSb and CoTiSb are as Ti: $3d^2\ 4s^2$, Fe: $3d^6\ 4s^2$, Co: $3d^7\ 4s^2$ and Sb: $5s^2\ 5p^3$respectively.

III. Results And Discussion

1.1 Ground State Properties

The lattice constants are optimized and the total energy is calculated for FeTiSb and CoTiSb alloys in nonmagnetic and magnetic phases. The calculated ground state properties such as equilibrium volume (V_0), lattice constant (a), valance electron density (ρ), bulk modulus (B_0),bulk modulus derivative (B') and Fermi energy (E_F) for FeTiSb and CoTiSb for are given in Table 1 along with available results [5,6].

Table1. The equilibrium volume V_0 (Å^3), optimized lattice constant a (Å), Valence electron density ρ (electrons/ Å^3), bulk modulus B (GPa) and its derivative(B') and Fermi energy E_F (eV).

	FeTiSb		CoTiSb	
	NM	FM	NM	FM
V_0	51.890	52.980	50.980	50.980
			51.250[a]	
a	5.921	5.962	5.886	5.886
	5.893[b]	5.897[b]	5.838[b]	5.826[b]
		5.957[c]	5.884[c]	
ρ	0.327	0.327	0.353	0.353
B_0	124.705	101.859	122.517	122.518
B'	5.829	5.834	5.848	5.836
E_F	6.479	6.480	6.319	6.323

[a] Ref [5], [b] Ref [6], [c] Ref [7]

3.2 Structural Phase transition

The structural stability of FeTiSb and CoTiSb alloys of both nonmagnetic and magnetic phases is analyzed under normal and high pressure. The lattice constants are optimized and the total energy is calculated for both FeTiSb and CoTiSb alloys for nonmagnetic and magnetic phases as a function of cell volume and their values are given in Table 2. FeTiSb adopt the magnetic phase of cubic (CI_b) as the most stable structure whereas CoTiSb possess the nonmagnetic cubic (CI_b) structure which both have the symmetry of the F-43m (216) space group.

Table 2. Listed the nonmagnetic and magnetic energies (eV) of FeTiSb and CoTiSb alloys with function of cell volume (Å^3).

FeTiSb				CoTiSb		
Cell volume	NM	Cell volume	FM	Cell volume	NM	FM
51.89	-21.222856	52.98	-21.299408	50.98	-20.974511	-20.970342
46.69	-20.943192	47.68	-21.060186	45.86	-20.688471	-20.685324
41.50	-19.848984	42.37	-20.112599	40.78	-19.584768	-19.581713
36.32	-17.326899	37.07	-17.816728	35.68	-17.018782	-17.015265
31.12	-12.204462	31.79	-13.071123	30.58	-11.792953	-11.791505
25.94	-2.275234	26.49	-3.668979	25.48	-1.532873	-1.530629

3.3 Mechanical Properties

The elastic constants C_{ij}, bulk modulus B_0, bulk modulus derivative B', Young's modulus E, Energy gap E_g, Magnetic moment M, B/G ratio and Poisson's ratio (ν) for the stable phase of FeTiSb and CoTiSb alloys are listed in Table 3. The calculated Young's modulus and bulk modulus of both the alloys indicates that CoTiSb is stiffer and stronger capacity to resist deformation than FeTiSb. The larger Poisson's ratio value clearly indicates that ionic contribution is dominant in XTiSB (X= Fe, Co) alloys. The calculated (B/G) values of XTiSb (X= Fe, Co) alloys show that both FeTiSb and CoTiSb alloys posses the brittle nature at zero pressure.

3.4 Electronic properties

The spin polarized and total density of states (DOS) of FeTiSb and CoTiSb is given in Fig.1 (a) & (b) and Fig. 2 (a) & (b) respectively. The peaks observed at lower energy region is due to the Fe-3d, Co- 3d and Sb-5s states, and the peaks at higher energy region are due to the 3d states of Ti. In Fig 1(a) shows that there is no symmetry between spin up (↑) and spin down (↓) of the spin polarized DOS of FeTiSb, which clearly explains that FeTiSb exhibits the half metallic nature with an energy gap of 0.576 eV. In Fig 2(a) spin up (↑) and spin down (↓) of the CoTiSb posses the symmetry nature. [7]. In CoTiSb alloy, Sb atom has five valence electrons and Co and Ti totally have 13 valence electrons. Among these 13 transition metal electrons only three are catched by the Sb atom and the remaining 10 electrons occupy the bonding d states. So, CoTiSb is a semiconductor with an energy gap of 1.013 eV.

Table 3. Listed the elastic constants C_{ij} (GPa), bulk modulus B_0 (GPa), bulk modulus derivative B'(GPa), Young's modulus E (GPa), Energy gap E_g (eV), Magnetic moment M (μ_B), B/G ratio and Poisson's ratio (ν) for the stable phase of FeTiSb and CoTiSb alloys.

	C_{11}	C_{12}	C_{44}	B_0	B_0'	E	E_g	M	B/G	ν
FeTisb (FM)	257.317	46.739	71.792	116.931 132.53[a]	5.834 4.95[a]	205.6345	0.576	0.906 0.82[a]	1.372	0.206
CoTiSb (NM)	269.856 259[c] 232[d]	77.416 84 [c]	76.242 93 [c] 77.4 [d]	141.56 142 [c] 129 [d]	5.848	210.876 224 [c]	1.013 0.95[b]	0.001	1.690 1.67 [d]	0.251 0.24 [c] 0.25 [d]

[a]Ref[6], [b] Ref[7], [c] Ref[8], [d] Ref[9]

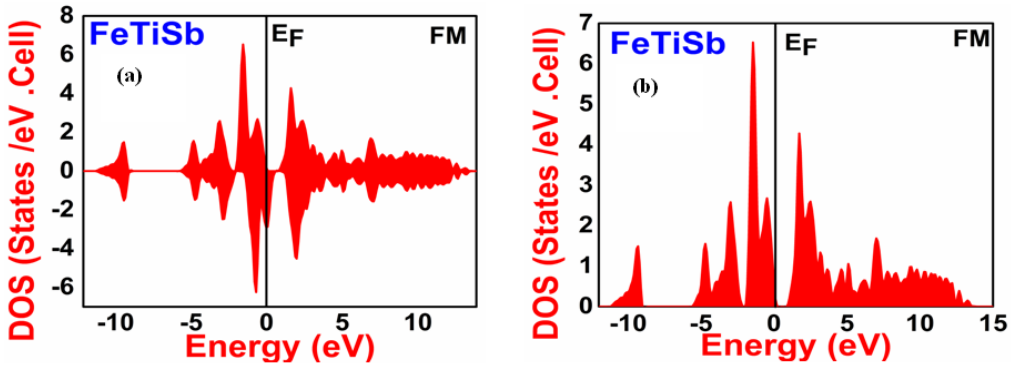

FIG .1. (a) & (b). spin up (↑) and spin down (↓) density of states and Total density of states of FeTiSb

3.5 Magnetic Properties

Non-spin and spin polarized calculations are performed to check the magnetic stability of both FeTiSb and CoTiSb alloys at ambient pressure. Table 2 indicates that the FeTiSb is stable in ferromagnetic phase (FM) and CoTiSb are stable in the nonmagnetic (NM) phase, and their corresponding magnetic moments are found to be 0.906 μ_B and 0.001 μ_B. The individual magnetic moment of Fe, Sb and Ti atoms are 1.195 μ_B 0.018 μ_B and -0.309 μ_B. at normal pressure. Ti atom shows the negative magnetic moment whereas Fe, sb atoms give the positive magnetic moment. The reduction of total magnetic moment of FeTiSb alloy is accompanied by the hybridization between the negative spin moments of Ti and the Fe and Sb atoms.

IV. Conclusion

In conclusion, first principles calculations have been performed using Vienna ab-initio simulation package with GGA-PBE to investigate the structural, electronic and mechanical properties of titanium based magnetic materials with two possible phases. FeTiSb is stable in ferromagnetic phase (FM) and CoTiSb is stable in the nonmagnetic (NM) phase phase. The calculated mechanical properties of FeTiSb and CoTiSb alloys say that the CoTiSb is the stiffer material than FeTiSb. The electronic structure reveals that FeTiSb having half metallic ferromagnets material at normal pressure. In CoTiSb alloy is a semiconductor. The magnetic moment of both FeTiSb and CoTiSb alloys are also estimated.

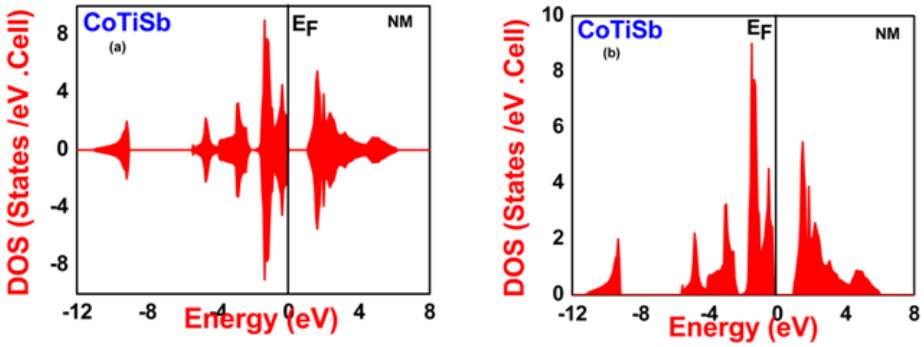

FIG .2.(a) & (b) spin up (↑) and spin down (↓) density of states and Total density of states of CoTiSb

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