Study of energy bands and magnetic properties of Co₂CrSi Heusler alloy

DIBYA PRAKASH RAI, SANDEEP, M P GHIMIRE and R K THAPA*

Department of Physics, Mizoram University, Aizawl 796 009, India

MS received 9 December 2010

Abstract. The electronic and magnetic properties of Co₂CrSi is calculated by using full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). Density of states (DOS), magnetic moment and band structures of the system are presented. For the exchange and correlation energy, local spin density approximation (LSDA+U) with the inclusion of Hubbard potential U is used. Our calculation shows indirect bandgap of 0.91 eV in the minority channel of DOS. This is supported by band structures and hence favoured the half metallic ferromagnetic (HMF) nature of the system. The effective magnetic moment of 4.006 μ_B also supported our conclusion with a near integral value. The DOS of Co and Cr were found to hybridize and was also responsible for the ferromagnetic nature of the system.

Keywords. FP-LAPW; LDA+U; DOS; magnetic moments; band structures.

1. Introduction

The Heusler compounds, as named after their discoverer are ternary intermetallics with a 2:1:1 stoichiometry and the chemical formula, X₂YZ. They usually consist of two transition metals X and Y and a main group element Z. Half-metallic ferromagnetism was first predicted for the half Heusler compound like NiMnSb by de Groot *et al* (1983). Half-metal ferromagnets (HMF) exhibit a real gap in minority density of states (DOS). Due to ferromagnetic (FM) decoupling, spin up bands are metallic and spin-down bands are semiconducting or *vice-versa*. In the present context of scientific research of material science, HMFs (Ghimire *et al* 2010) have become one of the most studied classes of materials. Consequently only charge carriers of one spin direction contributes to the conduction. The existence of a gap in the minority-spin band structure leads to 100% spin polarization of the electron states at the Fermi level, which makes the systems applicable for spintronic devices (Zutic *et al* 2004). In half-metals, the creation of a fully spin-polarized current should be possible that should maximize the efficiency of magnetoelectronics devices (de Boeck *et al* 2002). Materials with high spin polarization can be used for tunnel magnetoresistance (TMR) and giant magnetoresistance (GMR) (Yakushi *et al* 2006). This is due to a high Curie temperature beyond room temperature and a simple fabrication process such as d.c. magnetron sputtering in Co₂YZ (Y=Mn, Cr, Fe and Z=Al, Si, Ge, Ga) (Miura *et al* 2004). We intend to calculate the electronic and magnetic properties of Co₂CrSi

by using the FP-LAPW method. DOS, magnetic moments and band structures of these compounds are investigated and compared.

2. Calculation details and crystal structures of Heusler compounds

X₂YZ Heusler compounds crystallize in the cubic L_{21} structure with space group $Fm\bar{3}m$ as shown in figure 1. The cubic L_{21} structure consists of four inter-penetrating *fcc* sublattices, two of which are equally occupied by Co. The two Co-site *fcc* sublattices combine to form a simple cubic sublattice. First principles FP-LAPW method based on DFT (Kohn and Sham 1965) is used for Co₂CrSi. For the exchange-correlation potential, LSDA+U method (Anisimov *et al* 1997) is used. In the LSDA+U calculations, the on-site Coulomb energy, U and exchange parameter, J applied are 0.52 and 0.00 Rydberg (Ry), respectively. Since the transition *d*-state electron correlations are expected to be strong, LSDA+U method is used. The number of *k*-points used for optimization was 10000 and $R_{MT} \times K_{MAX}$ was taken as 7 for consistency. The muffin-tin sphere radii (RMT) used are 2.2, 2.0 and 1.89 a.u. for Co, Cr and Si, respectively. Self-consistency is achieved with energy convergence of 10^{-3} Ry. WIEN2k code (Blaha *et al* 2008) was employed for computations which was also used by Rai *et al* (2010).

X₂YZ Heusler compounds crystallize in the cubic L_{21} structure (space group, $Fm\bar{3}m$). The cubic L_{21} structure consists of four inter-penetrating *fcc* sublattices, two of which are equally occupied by Co. The two Co-site *fcc* sublattices combine to form a simple cubic sublattice.

* Author for correspondence (r.k.thapa@gmail.com)

Figure 1. Structure of Co_2CrSi Heusler alloy: Co (red) atoms are at origin and $(1/2, 1/2, 1/2)$, Cr (green) at $(1/4, 1/4, 1/4)$ and Si (blue) atoms at $(3/4, 3/4, 3/4)$.

3. Results and discussion

3.1 Density of states and magnetic moments

The partial DOS plots are shown in figure 2(a–d). From figure 2(a–b), peaks due to Co atoms are found mostly in the core, semi-core and the valence region below E_F for both spin channels due to its d state electrons. In spin up channel, the DOS cuts E_F showing the metallic nature shown in figure 2(a). In spin down channel, peaks are due to d states of Co atoms of the conduction region (figure 2(b)). A bandgap of 0.91 eV is observed with the Fermi level lying midway between the gap (figure 2(b)) in spin down channel showing semiconducting behaviour. The $3d$ electrons of Co atoms were decomposed into $d\text{-}eg$ and $d\text{-}t2g$ states (Galanakis *et al* 2002). In the conduction region of spin down, peaks were observed at 0.70 eV and 1.8 eV which is mainly due to $d\text{-}eg$ and $d\text{-}t2g$ states, respectively. We observe an exchange splitting between $d\text{-}eg$ up and down with a splitting energy of 1.4 eV. Also an exchange splitting of 2.6 eV was observed for $d\text{-}t2g$ up and down states (figure 2(a–b)). Similarly we observe that Cr atoms mainly contribute in the valence region with two sharp peaks at

Figure 2. Partial DOS of Co and Cr atoms.

Table 1. Experimental and theoretical values of lattice constants, magnetic moments, energy gaps and bulk modulus.

Compound	Lattice constant, a_0 (Å)		Magnetic moment, μ_B		Energy gap, E_g (eV)		k -value	Bulk modulus (GPa)
	Experimental	Theory	Previous	Observed	Previous	Observed		
Co ₂ CrSi	5.647 ^b	5.699	4.000 ^b	4.006	0.878 ^b	0.910	10,000	405.556

^bRaphael *et al* (2002)**Table 2.** Partial and total magnetic moments.

Previous calculation			Our calculation				Energy gap, E_g (eV)	
Magnetic moment, μ_B			Magnetic moment, μ_B					
Co	Cr	Total	Co	Cr	Si	Total	Previous	Our calculation
0.980	2.080	4.000 ^b	0.980	2.102	−0.055	4.006	0.878 ^b	0.910

^bRaphael *et al* (2002) **Figure 3.** (a) Energy band of Co₂CrSi for spin up, (b) total DOS of Co₂CrSi and (c) energy band of Co₂CrSi for spin down.

−1.4 eV and −2.0 eV due to Cr-*d* state electrons in spin-up configuration with a Fermi cut-off (figure 2(c)). In spin-down configuration, a 3*d* state electron of Cr contributes both in the valence and the conduction regions with an energy gap of 0.94 eV (figure 2(d)). Sharp peak at −0.8 eV is due to both *d-eg* and *d-t2g* states of Cr-3*d* atoms in spin-up channel (figure 2(c)). In spin-down channel, the peaks in the valence and conduction regions are due to both *d-eg* and *d-t2g* states of Cr atoms (figure 2(d)). An exchange splitting of 2.4 eV is observed between spin-up and spin-down channel due to the 3*d* states of Cr atoms. This splitting explains the higher value of magnetic moment in Cr atoms (table 1). The partial magnetic moments of the atoms Co, Cr and Si are 0.980 μ_B , 2.102 μ_B and −0.055 μ_B , respectively. Thus the total magnetic moment is 4.006 μ_B which is approximately an integer value of 4.00 μ_B (Kandpal *et al* 2006). The partial magnetic moments are tabulated and compared with the previous results as shown in table 2.

3.2 Band structure of Co_2CrSi

From figure 3 of the band structure the calculated energy gap along Γ -X symmetry is 0.91 eV which is almost similar to 0.878 eV (Kandpal *et al* 2006). The Cr compounds give comparatively high E_g compared to others as seen from DOS as well as from the band structure. The band gap is determined by the indirect bandgap.

4. Conclusions

We have calculated DOS, magnetic moments and band structures of Co_2CrSi using FP-LAPW method with LSDA+U approximation. The results were in support of the HMF nature of Co_2CrSi . The existence of energy gap in DOS for minority spins is an indication of Co_2CrSi being a poten-

tial HMF. This is also evident from the energy band results calculated. The calculated magnetic moment for Co_2CrSi is 4.006 μ_B which is in agreement with the integral value of 4.00 μ_B (Kandpal *et al* 2006) supporting the HMF nature of Co_2CrSi .

Acknowledgements

One of the authors (SD) acknowledges a research fellowship (JRF) and (RKT), a research grant from DAE, BRNS, Mumbai.

References

- Anisimov V I, Aryasetiawan F and Lichtenstein A I 1997 *J. Phys.: Condens Matter* **9** 767
- Blaha P, Schwarz K, Madsen G K H, Kvasnicka D, Luitz J and Schwarz K 2008 *An augmented plane wave plus local orbitals program for calculating crystal properties, Wien2K user's guide* (Wien: Tech Universitat Wien)
- de Boeck, van Roy W, Das J, Motsnyi V, Liu Z, Lagae L, Boeve H, Dessein K and Borghs G 2002 *Semicond. Sci. Technol.* **17** 342
- de Groot R A, Mueller F M, van Engen P G and Buschow K H 1983 *J. Phys. Rev. Lett.* **50** 2024
- Galanakis I, Dederichs P H and Papanikolaou N 2002 *Phys. Rev.* **B66** 174429
- Ghimire M P, Sandeep and Thapa R K 2010 *Mod. Phys. Letts* **B24** 2187
- Kandpal H C, Fecher G H, Felser C and Schonhense G 2006 *Phys. Rev.* **B73** 094422
- Kohn W and Sham L J 1965 *Phys. Rev.* **A140** 1133
- Miura Y, Nagao K and Shirai M 2004 *Phys. Rev.* **B69** 144413
- Rai D P *et al* 2010 *Indian J. Phys.* **84** 593
- Raphael M P *et al* 2002 *Phys. Rev.* **B66** 104429
- Yakushi K, Saito K, Takanashi K, Takahashi Y K and Hondo K 2006 *Appl. Phys. Lett.* **88** 082501
- Zutic I, Fabian J and Sharma S D 2004 *Rev. Mod. Phys.* **76** 323