Fermi Surface Studies Of Co-based Heusler Alloys: Ab-initio Study

Swetarekha Ram, V. Kanchana*

*Department of Physics, Indian Institute of Technology Hyderabad, Ordnance Factory Estate, Yeddumailaram-502205, Andhra Pradesh, India, *Email:kanchana@iith.ac.in*

Abstract. The electronic, Fermi surface (FS) and magnetic properties of ferromagnetic Heusler alloys Co_2XY (X = Cr, Mn, Fe; Y=Al, Ga) have been investigated by means of first principles calculation. Out of these compounds, Co_2CrAl is found to be perfectly half-metallic (HM) at ambient. Under pressure HM to nearly HM (NHM) transition is observed around 75 GPa for Co_2CrAl and NHM to HM transition is observed around 40 GPa and 18 GPa for Co_2CrGa and Co_2MnAl, respectively, while no transition is observed for other compounds under study and is also analyzed from the FS studies. The states at the Fermi level in the majority spin are strongly hybridized Co-d and X-d like states. The majority band FS topology change is observed under pressure for the compounds where we observe a transition, while the minority band FS remain unaltered under pressure for all compounds except in Co_2FeGa, where we observed an electron sheet at X point instead of hole pocket at Γ point.

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INTRODUCTION

The Co-based Heusler alloys have a great attention due to their high Curie temperature [1]. Theoretically it was predicted that most of Co-based Heusler alloys behave like HM, where they are expected to provide 100% spin-polarization at Fermi level (E_F) [2]. These half-metallic ferromagnetic materials can be used as a perfect spin filters or to enhance the performance of spin-dependent devices. Inspite of these, there are many discrepancies in the electronic properties of these compounds. Ishida et. al [3] have shown that Co_2CrAl has a complete spin polarization at the E_F which contradicts the prediction of Galanakis [4]. Co_2XY type Heusler alloys are good candidates for spintronics materials, where X atoms belong to transition metal and Y is a main group element.

METHOD OF CALCULATION

We have carried out density functional calculations using the full potential linear augmented plane wave method. For the exchange-correlation functional, the generalized gradient approximation (GGA) was used. The self-consistent calculations were considered to be converged when the total energy of the system was stable within 10^{-6} Ry. A (44×44×44) mesh was used for the Fermi surface calculations to ensure accurate determination of the E_F.

Results And Discussion (Band Structure, Fermi Surface And Density Of States)

We have calculated the density of states ($N(E_F)$) for minority ($\downarrow$) and majority ($\uparrow$) spin and the spin polarization (SP) ratio at E_F and are reported in TABLE 1, which confirm Co_2CrAl to be a perfect HM with 100% SP at E_F, while Co_2CrGa, $Co_2MnAl(Ga)$, $Co_2FeAl(Ga)$ are NHM with SP less than 100%. The observed NHM nature of these compounds is mainly due to the valence band maximum (VB_{max}) crossing the E_F and forming three hole pockets at the Γ point for corresponding three bands (FIGURE 1(a, b)) which are Co-d (t_{2g}) like states except in Co_2FeAl, where we found the conduction band minimum (CB_{min}) to cross the E_F at X point, thereby forming an electron pocket (FIGURE 1(c, d)) and is mainly Fe-d(e_g) like states. The presence of the hole or electron pocket for minority spin band with finite value of $N(E_F)$ as reported in TABLE 1, further confirm the NHM behavior of these compounds, except Co_2CrAl, which is completely HM with zero $N(E_F)$ for the minority band. The majority spin band of all compounds are strongly metallic in nature and are hybridized Co-d

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and X-d orbitals with small contribution from Al(Ga)-p like states and is again reflected in the FS topology. The FS topology remains unchanged by replacing Al with Ga, which indicates the minimum contribution of Al(Ga) at E_F, but the FS topology do change when we vary the X(Cr, Mn, Fe) atom (FIGURE 2(a, c)).

FIGURE 1. (a, b) Minority spin band structure and FS of Co_2CrGa. The topology of other two surfaces is also same as 1st surface. In addition the topology for $Co_2MnAl(Ga)$ and Co_2FeGa is also same as Co_2CrGa; (c, d) Minority spin band structure and FS of Co_2FeAl.

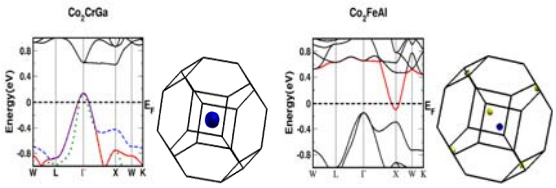
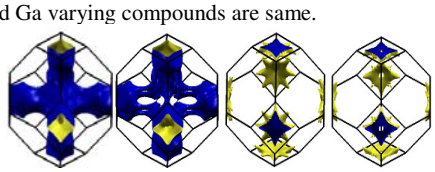
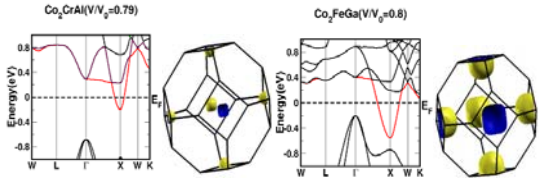


FIGURE 2. Majority spin FS, (a, c) for Co_2CrAl and Co_2MnAl at ambient; (b, d) under pressure. The topology of Al and Ga varying compounds are same.



Under pressure at nearly 75GPa, the HM behavior of Co_2CrAl is destroyed due to the downward shift of the band at X point, resulting in an electron pocket at X point in minority spin as shown in FIGURE 3(a). Similarly around 18GPa and 48GPa, Co_2CrGa and Co_2MnAl behave like a HM due to the downward shift of the band at Γ point, resulting in the vanishing of hole pocket for the minority spin band. The NHM nature of the other investigated compounds remains unaltered and the FS topology is also found to be the same under pressure. In addition to this, we observed an electron pocket at X point instead of hole pocket at Γ for Co_2FeGa due to the downward shifts of the band which is mainly Fe-d(e_g) like states and is evident from FIGURE 3(b). The main interesting feature of these investigated compounds is the observed FS topology change under pressure.

FIGURE 3. Variation of minority Band and FS under pressure, (a) Co_2CrAl (b) Co_2FeGa



We observe the majority band FS topology change for the compounds where transition is seen (HM to NHM in Co_2CrAl and NHM to HM in Co_2CrGa and Co_2MnAl) as shown in FIGURE 2. Though the topology of Co_2MnAl and Co_2MnGa are the same at ambient, the topology remains unaltered in Co_2MnGa, where we could not observe the magnetic transition till high pressure unlike Co_2MnAl.

CONCLUSION

Among all the compounds Co_2CrAl is found to be HM and turns NHM under pressure. The non-vanishing N (E_F) and the minority band FS confirm the NHM behavior of all these investigated compounds. The FS topology change for majority band is observed for the compounds where the transition from HM to NHM or NHM to HM state is observed.

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TABLE 1. Calculated $N(E_F)$ for majority (↑) and minority (↓) spin in (states/eV/spin) at the E_F, gap between CB_{min} and VB_{max}, spin polarization (SP) in % at the E_F, total magnetic moment in μ_B. All the calculated values are at zero pressure.

Compounds	$N(E_F\uparrow)$	$N(E_F\downarrow)$	SP	Gap in eV	μ_B(Total)
Co_2CrAl	4.12	0	100	0.73	3.00
Co_2CrGa	5.42	0.13	95.32	0.44	3.03
Co_2MnAl	1.02	0.15	74.64	0.67	4.04
Co_2MnGa	1.62	0.36	63.64	0.38	4.11
Co_2FeAl	0.87	0.08	83.94	0.05	4.99
Co_2FeGa	0.88	0.14	72.44	0.02	5.02