Review on Electronic and Magnetic properties of Fe–based full-Heusler compounds

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Abstract

Fascinating properties of Heusler alloys made these materials remarkably imperative for researchers. In this paper review on Fe-based full-Heusler compounds have been done. Electronic and magnetic properties of Fe2TiAl, Fe2VAl, Fe2CrAl, Fe2MnAl, Fe2CoAl and Fe2NiAl Heusler compounds have been reviewed. All calculations were based on FP-LAPW method implemented in wien2k code. Energy and correlation potential have been estimated by using GGA approximation for Fe2YAl (Y=Ti, V, Cr, Mn, Ni) compounds while GGA+U approximation has also been used for Fe2CoAl compound. Fe2YAl (Y=Ti, V, Co, Ni) Heusler compounds showed metallic behavior whilst Fe2CrAl and Fe2MnAl showed half-metallic behavior because of the energy gap in the spin down case. The magnetic moment for Fe2YAl (Y=Cr, Mn, Co, Ni) was obtained as 1 µB, 2.0013 1 µB, 4.90 1 µB, and 4.28319 1 µB respectively.

Keywords: Heusler compounds, Electronic properties, Magnetic properties.

Introduction

The materials formed by the composition of three elements are known as Heusler compounds and their name was given after the name of Fritz Heusler. He is the one who first invented these materials in 1903. Since then because of their surprising magnetic behavior research on these materials is increasing day by day. Cu2MnAl was the first Heusler compound, which showed ferromagnetic behavior despite the fact of no magnetic element was present in its composition [1, 2]. Therefore these materials become proficient aspirants for memory devices, thermoelectric materials, spintronics, spin-value generators & magneto resistive materials [3-6]. X, Y and Z elements in Heusler compounds are composite to form full (X2YZ) and half (XYZ) Heusler compounds, where X and Y are transition metals and Z is an s, p element [7, 8]. Full-Heusler compounds crystallize in L21 and XA structure [9]. Cu2MnAl (L21) and Hg2CuTi (XA) are two crystal type structures for full-Heusler compounds which lie under the space group number 225 known as Fm-3m and 216 known as F-43m respectively. For Fm-3m (SG) X, Y and Z positioned at (0.25, 0.25, 0.25), (0, 0, 0) and (0.5, 0.5, 0.5) in an order. In F-43m (SG) X contains two sites (0, 0, 0) and (0.25, 0.25, 0.25) designated as X1 and X2 while (0.5, 0.5, 0.5) and (0.75, 0.75, 0.75) are the atomic positions for Y and Z respectively [10]. Half-Heusler compounds crystallize in C1b structure. First half-Heusler compound investigated as a half-metallic compound was NiMnSb [11].
Fig.1: (a) is representing Hg$_2$CuTi structure and (b) is representing Cu$_2$MnAl type structure.

Half-metallicity is another unique property of Heusler compound, in which one spin has zero gaps at Fermi energy (E$_F$) while other spin shows insulating or semiconducting band gap. Therefore half-metallic Heusler compounds have 100% spin polarization. This property make them imperative candidate for spintronic devices, for instance magnetic tunnel junction (MTJ) or spin valves [12]. In this paper Fe-based Heusler compounds have been studied, which are investigated by using FP-LAPW [13] method that rely upon density functional theory (DFT) [14] and implemented in wien2k code [15]. Fe-based HCs attract great interest of researchers because there are number of compounds contain semiconducting or half-metallic nature.

Electronic properties

Electronic properties play very imperative role in predicting the half-metallic ferromagnetism. The behavior of electronic states near the Fermi level reveals the nature of compound. If these are crossing the Fermi level then compound has metallic nature or gap between them describe the insulating or semiconducting nature of compound. Attractive modulus, low density, fine environmental resistance, high thermal conductivity and melting temperature of Fe$_2$TiAl make it proficient aspirant for aeronautics and astronautics [16]. The calculated lattice parameter for Fe$_2$TiAl was 5.7788 Å in Fm-3m SG. Band structure of this compound confirmed the metallic behavior [17]. Some bizarre properties of Fe$_2$VAl were noticed [18]. Other studies suggested its non-magnetic behavior but contain super para-magnetic clusters and magnetic anti-site defects [19, 20]. The optimized lattice parameter for this compound was 5.6831 Å. Both spins for Fe$_2$VAl showed the same behavior not including any energy gap. Hence this did not show any ferromagnetic behavior and found to be nonmagnetic compound [17]. Fe$_2$CrAl show half-metallic behavior as density of states in minority spin showed pseudogap near the Fermi level. The equilibrium lattice constant for Fe$_2$CrAl was 5.610 Å. The electronic states shifted toward the higher binding energy in a majority spin
which results in a pseudo-gap at the Fermi level [17]. The above three HCs have also been investigated experimentally [21]. In Fe₂YAl (Y=Ti, V, Cr) HCs Al (s) density of states were found to be in the energy range -8 eV to -6 eV and Al (p), Fe (d) & Y (d) were responsible for the lowest scattered states. Sharma et al. showed that electronic, magnetic and optical properties of compounds got change by means of atomic configuration of HCs [17]. Fe₂MnAl and Fe₂NiAl investigated by F Dahmane et al. by considering Fm-3m and F-43m space group by using optimized lattice parameter 5.64 Å in Fm-3m and 5.65 Å in F-43m SG for Fe₂MnAl and 5.68 Å in Fm-3m and 5.67 Å in F-43m SG for Fe₂NiAl. The compound with Mn as Y found to be half-metallic in the Fm-3m SG and metallic in the F-43m SG. Band gap of 0.49 eV in the electronic states of minority spin validated the half-metallic character of Fe₂MnAl. Fe (d) and Mn (d) are the partial density of states responsible for the semiconducting behavior. The compound with Ni as Y was found to be metallic in both the cases as electronic states were crossing the Fermi level [22]. Investigation of Fe₂CoAl was done by considering L₂₁ and XA phases and found to be stable in XA phase. Different magnetic phases were also taken into account, for instance paramagnetic, ferromagnetic and antiferromagnetic phase from which ferromagnetic phase occurred as a stable phase. The compound showed metallic behavior with generalized gradient approximation (GGA) in both phases but showed a small energy gap of 0.87 eV in minority spin but at 0.5 eV above the Fermi level with GGA+U approximation, where Hubbard parameter (U) was set to 4.35 eV and 4.22 eV for Fe and Co respectively, which results in a metallic behavior of Fe₂CoAl [23].

### Table 1: Observed Electronic properties and net magnetic moment.

<table>
<thead>
<tr>
<th>Compound name</th>
<th>Electronic property</th>
<th>Magnetic moment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe₂TiAl</td>
<td>Metallic</td>
<td>-</td>
</tr>
<tr>
<td>Fe₂VAl</td>
<td>Metallic</td>
<td>0 µB</td>
</tr>
<tr>
<td>Fe₂CrAl</td>
<td>Half-metallic</td>
<td>1 µB</td>
</tr>
<tr>
<td>Fe₂MnAl</td>
<td>Half-metallic</td>
<td>2.0013 µB</td>
</tr>
<tr>
<td>Fe₂CoAl</td>
<td>Metallic</td>
<td>4.90 µB</td>
</tr>
<tr>
<td>Fe₂NiAl</td>
<td>Metallic</td>
<td>4.28319 µB</td>
</tr>
</tbody>
</table>

### Magnetic Properties

The calculated magnetic moment should also be reliable with the Slater-Pauling rule. It suggests that total magnetic moment should be equal to Nᵥ-24, where Nᵥ is number of valence electrons [24, 25]. The obtained value of magnetic moment for Fe₂VAl was 0 µB, whereas 1µB for Fe₂CrAl which were reliable with the Slater-Pauling rule [17]. Fe₂MnAl has 26 valence electrons which led to the integer value (2 µB) of magnetic moment and were reliable with the obtained value which is 2.0013 µB. In both Hg₂CuTi and Cu₂MnAl structures, Fe₂NiAl had no integer value
of magnetic moment which signified it to be metal [22]. The total magnetic moment of Fe$_2$CoAl was not consistent with SP rule and was not an integer [23].

Conclusion

Six Heusler compounds have been reviewed and two of them found to be half-metallic whilst other four found to be metallic. Fe$_2$TiAl & Fe$_2$VAl were stable in Cu$_2$MnAl structure and were metallic in nature. Fe$_2$CrAl & Fe$_2$MnAl were half-metallic in nature and achieved magnetic moment for them was 1 $\mu_B$ and 2.0013 $\mu_B$ respectively. These also were stable in Cu$_2$MnAl structure. Fe$_2$CoAl and Fe$_2$NiAl were metallic in nature and values of magnetic moment were 4.90 $\mu_B$ and 4.28319 $\mu_B$ in a row, whereas former is stable in Hg$_2$CuTi structure and latter in Cu$_2$MnAl structure.

References


