A Ground State Study of Structural and Magnetic Properties of Co$_2$CrGe: A GGA Method

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ABSTRACT

The structural and magnetic properties of Co$_2$CrGe, a Heusler alloy have been evaluated by first principles density functional theory through total energy calculations at 0 K by the full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K code. The calculated results were compared with the previously reported results. Generalized gradient approximation (GGA) was used to study the structural and magnetic properties of Co$_2$CrGe.

Key words: Magnetic properties, Heusler alloy, Total energy.

INTRODUCTION

Heusler alloys are the ternary intermetallic compounds with composition X$_2$YZ, where X and Y are transition elements (Ni, Co, Fe, Mn, Cr, Ti, V etc.) and Z is III, IV or V group elements (Al, Ga, Ge, As, Sn, In etc.). One of the promising classes of materials is the half-metallic ferrimagnets, i.e., compounds for which only one spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at $E_F$. After that, half-metallicity attracted much attention because of its prospective applications in spintronics. The electronic and magnetic properties of Co$_2$MnAl and Co$_2$CrSi using LSDA shows the half-metallicity at the ground state. In this paper, we have studied the various ground state and structural properties of Co$_2$CrGe using full potential linearized augmented plane wave (FP-LAPW) method within GGA.

Crystal structure

Heusler alloy with chemical formula X$_2$YZ (X = Co, Y = Cr and Z = Ge). The full Heusler structure consists of four penetrating fcc sublattices with atoms at X1(1/4,1/4,1/4), X2(3/4,3/4,3/4), Y(1/2,1/2,1/2) and Z(0,0,0) positions which results in L2$_1$ crystal structure having space group Fm-3m.

Computation detail

A computational code (WIEN2K) based on FP-LAPW method was applied for structure calculations of Co$_2$CrGe. GGA was used for the exchange correlation potential. The multipole expansion of the crystal potential and the electron density within muffin tin (MT) spheres was cut at $l=10$. Nonspherical contributions to the charge density and potential within the MT spheres were considered up to $l_{\text{max}}=6$. The cut-off parameter was $R_{\text{K_{max}}}=7$. In the interstitial region the charge density and the potential were expanded as a Fourier series with wave vectors up to $G_{\text{max}}=12$ a.u$^{-1}$. The MT sphere radii used were 2.35 a.u. for Co, 2.35 a.u. for Cr and 2.21 a.u. for Ge. The number of k-points used in the irreducible part of the brillouin zone is 286.

RESULTS AND DISCUSSION

The calculated total energies within GGA as function of the volume were used for determination of theoretical lattice constant and bulk modulus. Equilibrium lattice constant,
Table 1: Lattice parameters and Bulk modulus

<table>
<thead>
<tr>
<th>Lattice constant $a_0$ (Å)</th>
<th>Bulk Modulus (GPa)</th>
<th>Equilibrium Energy (Ry)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Previous</td>
<td>Our Calculation</td>
<td></td>
</tr>
<tr>
<td>5.740$^{[10]}$</td>
<td>5.7702</td>
<td>250.438</td>
</tr>
</tbody>
</table>

Table 2: Partial magnetic moments and energy gap of Co$_2$CrGe

<table>
<thead>
<tr>
<th>Previous Magnetic Moment ($\mu_B$)</th>
<th>Our Calculation</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
<tr>
<td>Previous</td>
<td>Our Calculation</td>
</tr>
<tr>
<td>Co</td>
<td>0.9321</td>
</tr>
<tr>
<td>Cr</td>
<td>2.1221</td>
</tr>
<tr>
<td>Ge</td>
<td>-0.0296</td>
</tr>
<tr>
<td>Total</td>
<td>3.999</td>
</tr>
</tbody>
</table>

Fig. 1: Co (yellow), Cr (blue) and Ge (pink)

Fig. 2: Energy as a function of volume

Fig. 3: Enthalpy versus pressure

Fig. 4: volume compression ratio versus pressure
isothermal bulk modulus, its pressure derivative are calculated by fitting the calculated total energy to the Murnaghan’s equation of state\(^9\).

The plot of energy versus volume is shown in Fig 2. The volume with respect to the lowest energy as shown in fig. 2 is used for determination of equilibrium lattice constant. The calculated values of lattice constant and bulk modulus are presented in Table 1. The calculated bulk modulus is 250.4376 GPa and its pressure derivative is found to be 7.4730. The optimized lattice constants for Co\(_2\)CrGe is 5.7702 which is presented. The change in the lattice constant of Co\(_2\)CrGe with that of previous result is 0.53% more. The enthalpy of the system was calculated by using the equation (H),

\[ H = E + PV \]  

where P is the bulk pressure, V is bulk volume and E is the Energy of the system. The plot of enthalpy versus Pressure is depicted in Fig. 3. Fig. 3 shows the enthalpy (H) is increasing and finally reaches stable volume 324.0732 \text{a. u}^{-3} at -9452.0364 Ry. In Fig. 4 it is shown the isothermal equation of states was obtained as a function of the volume compression ration \( V/V_0 \), where V and \( V_0 \) are the compressed and uncompressed volumes, respectively. The volume derivative decreases with the increase in pressure.

### Magnetic properties

The effective magnetic moment is 3.999\(\mu_B\) which is approximately an integer value 4.00 \(\mu_B\). The partial magnetic moments of Co, Cr and Ge atoms are 0.9321\(\mu_B\), 2.1221 \(\mu_B\) and -0.0296 \(\mu_B\) respectively. In the case of small magnetic moment compounds, the Co atoms contribute mostly to the moment, as compared with the compounds with large magnetic moments\(^11\). It should be noted that \(M_{\text{tot}}\) is the total magnetic moment but it is not the sum of the moments of Co, Mn and Z sites only, it also includes the moment of interstitial between the sites. In most cases the moment of Z (Ge) atoms aligned anti-parallel to the X(Co) and Y(Cr) moments as shown in Table 2. In our calculation we obtained the integral value of magnetic moment 3.999 \(\mu_B\) when the system is treated with GGA. This proves that the system Co\(_2\)CrGe treated with GGA can be possible half metal ferromagnet (HMF).

### CONCLUSION

The ground state structural optimization was performed to obtain the equilibrium energy. We have studied the possibility of appearance of half-metallicity in the case of the full Heusler compounds Co\(_2\)CrGe, where Ge is a sp atom belonging to the IVB column of the periodic table. We found that in Co\(_2\)CrGe the ferromagnetic is stable at the equilibrium lattice constant. The calculated value of magnetic moment is 3.999 \(\mu_B\) which is in qualitative agreement with the previously reported result\(^10\). The integral value of magnetic moment is one of the evidences to prove the Half Metallic Ferromagnet nature for Co\(_2\)CrGe.

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### REFERENCES

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