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Study of the structural properties of Co2YGe (Y=Sc, Ti, V, Cr, Mn, Fe) by GGA method

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ABSTRACT

The structural properties of Co2YGe, 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 properties of Co2YGe. The calculated values of lattice parameters were in qualitative agreement with the previously reported results.

Key words: GGA; FP-LAPW; structural properties; Wien2k.

INTRODUCTION

Heusler alloys are the ternary intermetallic compounds with the composition X_2YZ, 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[1] at E_F. After that, half-metallicity attracted much attention,[2] because of its prospective applications in spintronics.[3] The electronic and magnetic properties of Co_2MnAl and Co_2CrSi,[4,5] using LSDA shows the half-metallicity at the ground state.

Rai and Thapa have also investigated the electronic structure and magnetic properties as well as structural properties of Like Co_2MnGe, Co_2MnSn, Co_2CrAl and Co_2CrGa Heusler compounds by using a first principle study and reported HMFs.[6,7] High pressure research on structural or electronic phase transformations and behaviour of materials under compression based on their calculations or measurements have become quite interesting in the recent few years; as it provides insight into the nature of the solid state theories, and determine the values of fundamental parameters[8]. In this paper, we have studied the various ground state and structural properties of Co_2YGe using full potential lin-

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earized augmented plane wave (FP-LAPW) method within GGA.

Heusler alloys[9] are with chemical formula X_2YZ (X = Co, Y and Z = Ge) and the full Heusler alloys crystallize in the cubic $L2_1$ structure (space group Fm-3-m). The X atoms are placed on 8*a* X (1/4,1/4,1/4), 4*a* Y (1/2,1/2,1/2) and 4*b* Z (0,0,0) positions. The cubic $L2_1$ crystal structure consists of four inter-penetrating *fcc* sub-lattices, two of which are equally occupied by X. The two X *fcc* sub-lattices combine to form a simple cubic sub-lattice. The Y and Z atoms occupy alternatively the center of the simple cubic X_2 sub-lattice resulting in a CsCl type super structure. The crystal structure of Co_2YGe Heusler compounds is illustrated in Figure 1.

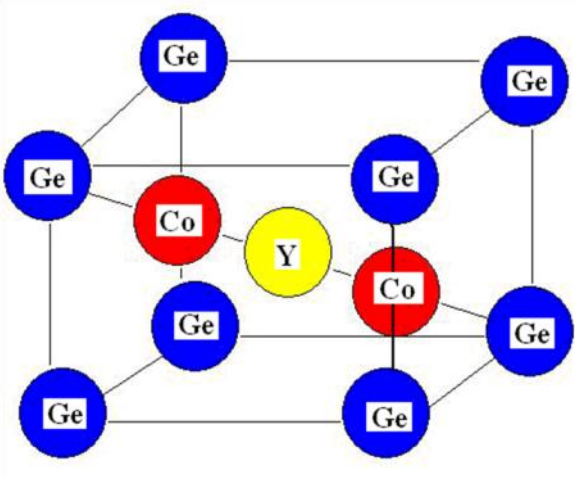

Figure 1. Co (red), Y (yellow) and Ge (blue).

THEORY AND COMPUTATIONAL DETAILS

The calculated total energies (E) within GGA as function of the volume (V) were used for determination of theoretical lattice constant and bulk modulus. Equilibrium lattice constant, isothermal bulk modulus, its pressure derivative are calculated by fitting the calculated total energy to the Murnaghan's equation of state.[10] A series of total energy calculations as a function of volume can be fitted to an equation of states according to Murnaghan.

$$E(V) = E_0 + \left[\frac{(V_0/V)^{B_0'}}{B_0' - 1} + 1\right] - \frac{B_0 V_0}{B_0' - 1} \qquad (1)$$

where E_0 is the minimum energy at T = 0K, B_0 is the bulk modulus at the equilibrium volume and B'_0 is pressure derivative of the bulk modulus at the equilibrium volume. The equilibrium volume is given by the corresponding total energy minimum as shown in Figure 2.[11]

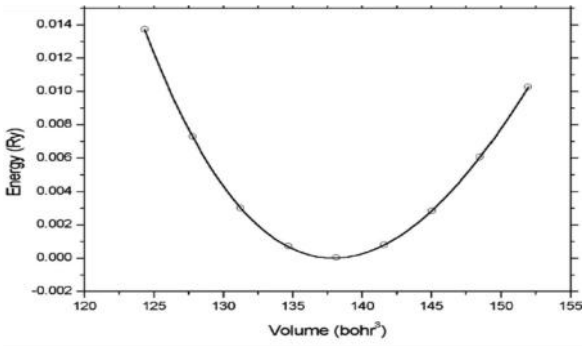

Figure 2. Total energy of TiC as a function of volume.[10]

Pressure, $P = -\frac{dE}{dV}$

Bulk modulus, $B_0 = -V\frac{dP}{dV} = V\frac{d^2E}{dV^2}$

A computational code (WIEN2K)[12] based on FP-LAPW method was applied for structure calculations of Co_2YGe. GGA[13] 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_{max}=6. The cut-off parameter was RK_{max}=7. In the interstitial region the charge density and the potential were expands as a Fourier series with wave vectors up to

Table 1. Muffin Tin Radius (RMT).

RMT (a. u)	Compounds					
	Co_2ScGe	Co_2TiGe	Co_2VGe	Co_2CrGe	Co_2MnGe	Co_2FeGe
Co	2.43	2.39	2.36	2.35	2.34	2.34
Y	2.43	2.39	2.36	2.35	2.34	2.34
Ge	2.29	2.24	2.21	2.21	2.20	2.20

Table 2. Lattice parameters and Bulk modulus.

Compounds	Lattice Constants a_o (Å)			Bulk Modulus B(GPa)	Equilibrium Energy (Ry)
	Previous	Calculated	$\Delta(a_o)$		
Co_2ScGe	5.953[14]	5.978	0.025	109.969	-11300.629
Co_2TiGe	5.842[14]	5.867	0.025	200.378	-11479.814
Co_2VGe	5.766[14]	5.792	0.026	202.158	-11670.736
Co_2CrGe	5.740[14]	5.770	0.030	250.438	-11873.835
Co_2MnGe	5.738[14]	5.749	0.011	219.479	-12089.405
Co_2FeGe	5.739[14]	5.758	0.019	162.677	12317.674

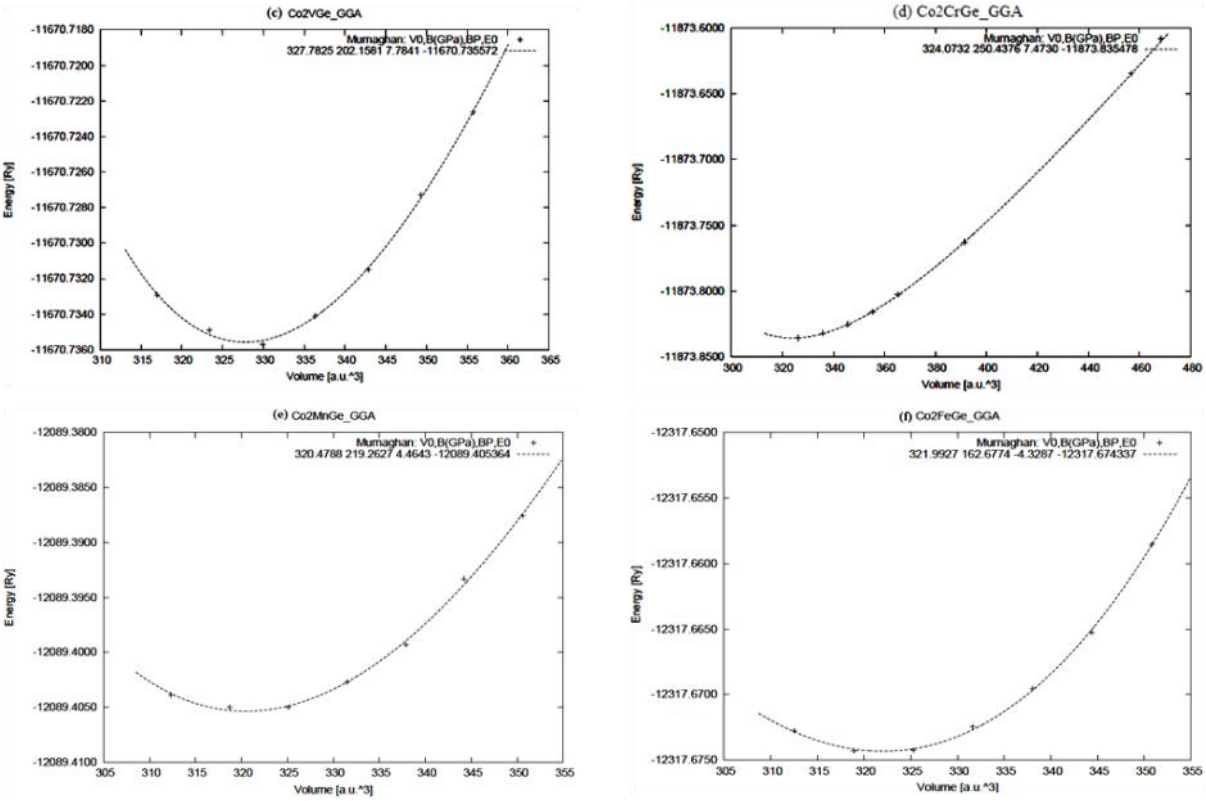

Figure 3. Energy as a function of volume.

G_{max}=12 a.u^{-1}. The Muffin Tin sphere radii (RMT) are given in Table 1. The number of k-points used in the irreducible part of the brillouin zone is 286.

Results and Discussions

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, isothermal bulk modulus, its pressure derivative are calculated by fitting the calculated total energy to the Murnaghan's equation of state given in Eq. (1). The plot of energy versus volume is shown in Figure 3. The volume corresponds to the lowest energy is used to determination of equilibrium lattice constant. The calculated values of lattice constant and bulk modulus are presented in Table 2.

The change in the optimized lattice constant of Co_2YGe with that of previous result is given as $\Delta(a_o)$. The enthalpy (H) of the system was calculated by using the Eq. (2),

$$H = E_0 + PV_0 \quad (2)$$

where P is the bulk pressure, V_o is bulk volume corresponds to minimum energy (E_o) of the system. The calculated enthalpy (H), pressure (P) and volume (V_o) is depicted in Table 3.

Kandpal *et al.* has reported the ferromagnetic configuration is lower in energy than the non-spinpolarized case.[15] We have also found the same trend where the energy is minimum for the highest ferromagnetic compound, i.e. Co_2FeGe and the energy is maximum for lowest ferromagntic compound Co_2ScGe as shown in Figure 4. The minimum of the total energies of the phases with E(Co_2FeGe) < E(Co_2MnGe) < E(Co_2CrGe) < (Co_2VGe) < E(Co_2TiGe) < E(Co_2ScGe) rank indicates that Co_2FeGe is the most stable structure as it was reported in the case of ScN.[16] According to Figure 4, the lowest enthalpy is observed at the low ferromagnetic compound Co_2ScGe as well as in strong ferromagnetic compound

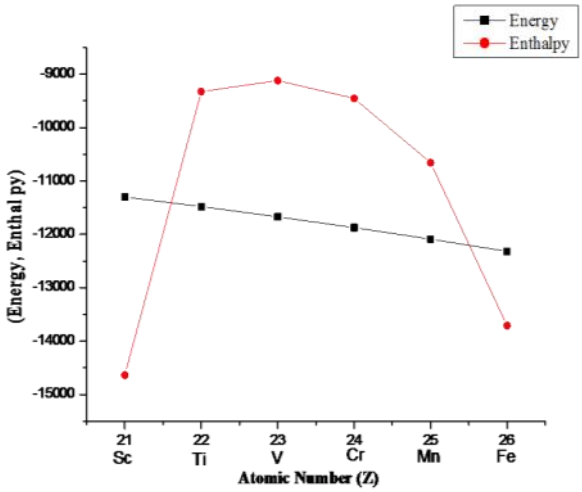

Figure 4. Plot of energy and enthalpy against valence electron (Z).

like Co_2FeGe. It is also seen in Figure 4 that there is a slow variation of enthalpy as we move from Co_2TiGe to Co_2MnGe which predicts the stability of bulk modulus shown in Table 2.

Conclusion

The ground state structural optimization was performed to obtain the equilibrium energy. The optimize Lattice parameters of the full Heusler compounds Co_2YGe, where Ge is a *sp* atom belonging to the IVB column of the periodic table were compared with the previously available results. The calculated values of lattice parameters were in qualitative agreement with the previously reported results.[14] We have also calculated the enthalpy (H) of the system. The sharp variation of enthalpy was noticed for high and low ferromagnetic compounds like Co_2FeGe and Co_2ScGe respectively. The minimum of the total energies of the phases with E(Co_2FeGe) < E(Co_2MnGe) < E(Co_2CrGe) < E(Co_2VGe) < E(Co_2TiGe) < E(Co_2ScGe) rank indicates that Co_2FeGe is the most stable structure as it was reported in the case of ScN.[16]

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