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Structural, electronic and magnetic properties of quaternary Heusler compounds CoYFeZ and CoYMnZ (Z = Si, Ge, Ga and Al): An ab-initio Study

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Abstract

We have studied electronic and magnetic structural properties of quaternary Heusler alloys CoYXZ where X is a transition metal with 3d electrons (X=Fe and Mn) and Z is the main group element (Z = Si, Ge, Ga and Al). These calculations were performed by an ab-initio study based on the density functional theory (DFT) approach. We searched the most stable structure of our materials studied among three possible arrangements (type-1, type-2, type-3). The structural stability of quaternary Heusler CoYXZ alloys (X = Fe and Mn, Z = Al, Si, Ga and Ge) was studied by the calculation of their cohesion and phonon energies. The type-1 structure is found energetically the most stable. According to our study, the quaternary Heusler CoYMnGa and CoYMnAl alloys proves to be a half-metal ferromagnetic with a total magnetic moment of 4.00μ_B. While the quaternary Heusler CoYMnGe and CoYFeZ (Z=Al, Si, Ge and Ga) alloys, seem to be not ferromagnetic, with zero moment magnetic. The quaternary Heusler CoYMnSi and CoYMnGe alloys are found ferromagnetic with magnetic moment of 1.91 μ_B and 2.90 μ_B respectively. In addition, it is also divulged that half-metallicity in these compounds is closely related to arrangements of magnetic atoms in Heusler alloys. The magnetization of the compounds CoYFeZ and CoYMnZ comes mainly from the 4d electrons the of Yttrium (Y) atom and the 3d electrons of the Fe and Mn atoms.

Keywords: Quaternary Heusler alloy; Half-metallic ferromagnetism; Electronic structures; Density functional theory.

1. Introduction

In recent decades, the extraordinary evolution of spin electronics has led to intense research activity in a new class of half metallic ferromagnetic materials. Indeed, since the prediction of half metallicity [1], the scientific interest of half-metallic ferromagnetic materials and has generated considerable theoretical and experimental. The most adopted strategies currently used to achieve this objective are based mainly on doping semiconductors with transition-metal impurities [2, 3, 4] and with non-magnetic [5, 6, 7, 8]. Many efforts have been made to study the CoYXZ quaternary Heusler alloys, where Y is yttrium, X (X=Fe and Mn) and (Z = Si, Ge, Ga and Al). The quaternary Heusler compounds crystallize in the cubic structure (F-43 m, space group No. 216) with LiMgPdSn as prototype [9, 10]. There are three possible structure types. In the first structure, denoted type-1, atoms Co, Y and X occupy respectively the positions (3/4, 3/4, 3/4), (1/2. 1/2. 1/2) and (1/4. 1/4. 1/4). The second structure, denoted type-2, the Co, Y and X atoms occupy respectively the positions (3/4, 3/4, 3/4), (1/4. 1/4. 1/4) and (1/2. 1/2. 1/2). For the third configuration, denoted type-3, atoms Co, Y and X respectively occupy the sites (1/2. 1/2. 1/2), (3/4, 3/4, 3/4) and (1/4. 1/4. 1/4). Note finally that in the three types of structure, the element Z (Z = Si, Ge, Ga and Al) is fixed at position (0, 0, 0). Many efforts have been made to study new quaternary Heusler, such as the quaternary CoFeXZ (X = Ti, Z = Si, Ge and As) which adopts the crystalline structure of LiMgPdSn type. The electronic structure reveals that these materials are half metals at normal pressure whereas metals at high pressure. On the other hand, the calculated electronic and magnetic properties based on type-1, indicate that yttrium based quaternary Heusler alloys YCoCrZ (Z = Si, Ge, Ga, Al) alloys are half-metallic ferromagnetic [11]. CoFeCrGa and CoFeCrGe alloys have been shown to be nearly half-metallic ferromagnetic materials, YCoCrZ (Z = Si, Ge, Ga, Al) demonstrates that (Type-1) configuration is the most stable one. Whereas CoFeCrAl and CoFeCrSi alloys show a half-metallic ferromagnetic behavior [12]. Experimentally [13], it was also established that CoFeCrSi and CoFeCrGe alloys exhibited a half-metallic ferromagnetic. In contrast, a recent study [14] revealed that Ru-based Heusler alloys such as CoRuFeGe and CoRuFeSn alloys had a ferromagnetic half-metallic character while CoRuFeSi alloy was almost a ferromagnetic half-metallic material. However, other materials without transition metal elements have been

studied [15]. Most of the theoretical and experimental studies carried out on the quaternary Heusler are based on 3d transition metals such as CoFeMnZ (Z = Al, Ge, Ga, As, Sb) [16-17-18], CoFeCrZ (Z = Al, Ga, Si, Ge) [19-20-21], CoMnCrAl [22], NiFeTiZ (Z = Si, Ge, P) [23] and FeCrMnSb [24]. Recently, studies have been made on the Heusler quaternary based on 4d elements, such as CoRhMnZ (Z = Ga, Sn) [25], CoMnYZ (Z = Al, Ga, In) [26], CoRuFeZ (Z = Si , Ge, Sn) [27], CoRuTiZ (Z = Si, Ge, Sn) [28], YCoVZ (Z = Si, Ge) and YCoTiZ (Z = Si, Ge) [29]. Although today there are over a thousand Heusler quaternary compounds and new families of quaternary alloys have not been studied, in particular, the alloys CoYXZ (X= Fe and Mn; Z = Si, Ge, Ga and Al) where the chemical element Y is yttrium. These materials may have a half-metallic ferromagnetic character. To our knowledge, there is no theoretical and experimental work for these compounds. Only CoYFeSi alloy has been studied and found nonmagnetic in type-1 structure. In this study, we use a method based on the theory of functional density (DFT) to study these new quaternary Heusler

2. Computational details

We have performed a first-principles calculations within the generalized gradient approximation (GGA) [30] in a plane wave basis, with the ultrasoft Vanderbilt pseudopotentials [31], using a pseudo-potential plane-wave (PP-PW) method as implemented in the Quantum ESPRESSO code [32]. The cutoff energy for plane waves is chosen to 80 Ry and an energy cut-off of 400 Ry was included for the charge density. A Gaussian smearing of 0.02 Ry has been applied. The integration on the Brillouin zone was calculated within a 12×12×12 k-points Monkhorst-Pack [33] mesh. The phonon dispersive curves, using the phonon code of quantum-Espresso code, have been calculated on a 4×4×4q-point mesh of the first Brillouin zone to obtain eight dynamic matrices. Calculations proceeded self-consistently until the total energy converged to within 0.1 meV/cell. Finally we consider only the ferromagnetism case.

3. Results

3.1 Structural properties

The structure adopted in this work contains four atoms Co, Y, X (X = Fe and Mn) and Z (Z = Si, Ge, Ga and Al). According to the distribution of atoms, we can distinguish three types of possible structure (type-1, type-2 and type-3). In the type-1 structure, the atoms Co, Y and X respectively occupy the positions (3/4, 3/4, 3/4), (1/2, 1/2, 1/2) and (1/4, 1/4, 1/4). In the type-2 structure, the atoms Co, Y and X occupy the positions (3/4, 3/4, 3/4), (1/4, 1/4, 1/4) and (1/2, 1/2, 1/2) respectively. In the type-3 structure, the atoms Co, Y and X occupy the positions (1/2, 1/2, 1/2), (3/4, 3/4, 3/4) and (1/4, 1/4, 1/4) respectivelyNote that in the three structures, the element Z (Z = Al, Si, Ga and Ge) occupies the fixed position (0,0,0). The equilibrium structural parameters are obtained by minimizing the total energy E with respect to the volume. The structural parameters of the quaternary compounds to be determined are the mesh parameter structural (a_0) and the compression modulus (B_0). Finally, the Murnaghan state equation [34] is applied to determine the equilibrium energy E = E (V) and the pressure compression modulus. To define the most stable among types-1, type-2 and type-3 structure, the cohesion energy (E_{coh}) is calculated using the expression, $E_{coh} = E_{CoYXY} - (E_{Co} + E_Y + E_X + E_Z)$, where E_{CoYXY} is the total energy of the CoYXZ quaternary Heusler alloys and (E_{Co}, E_Y , E_X and E_Z) represent the total energies of the Co, Yttrium, X and Z respectively. The results of the structural optimizations, the cohesion energy and the total magnetic moments for CoX'XZ quaternary Heusler alloy given in Tables1 and 2 show that cohesion energy is minimal for type-1 structure, indicating that it is the most stable structure. Our calculations agree with recent first-principles calculations of CoYFeSi quaternary Heusler alloy [35]. The latter calculation finds that the type-1 structure is the most stable with a structural parameter of 6.08 Å.

Table1: The equilibrium structural parameter a(Å), the bulk modulus B(GPa), the cohesive energy E_{coh}(eV), the total magnetic moment M_{tot}(μ_B) per cell of CoYFeZ (Z= Al, Si, Ge and Ga) quaternary Heusler alloys.

CoYFeZ	Phase	a	B	E_{coh}	M_{tot}
CoYFeAl	Type-1	6.392	113.5	-17,16	-0.00
CoYFeAl	Type-2	6.417	86.1	-17,14	4.31
CoYFeAl	Type-3	6.353	105.3	-16,43	0.93
CoYFeSi	Type-1	6.084	146.7	-19,08	0.00
	Type-1	6.08[a]		-2.14	0.00
CoYFeSi	Type-2	6.333	102.0	-18,43	4.35
CoYFeSi	Type-3	6.190	176.8	-18,53	0.50
CoYFeGe	Type-1	6.169	130.8	-18,00	0.00
CoYFeGe	Type-2	6.413	98.3	-17,74	4.36
CoYFeGe	Type-3	6.436	94.2	-17,83	4.43
CoYFeGa	Type-1	6.353	128.8	-16,66	-0.00
CoYFeGa	Type-2	6.417	97.6	-16,60	4.42
CoYFeGa	Type-3	6.448	93.6	-16,63	4.52

[a]Reference [35]

Table 2 : The equilibrium structural parameter a(Å), the bulk modulus B(GPa), the cohesive energy E_{coh}(eV), the total magnetic moment M_{tot}(μ_B) per cell of CoYMnZ (Z= Al, Si, Ge and Ga) quaternary Heusler alloys.

CoYMnZ	Phase	a	B	E_{coh}	M_{tot}
CoYMnAl	Type-1	6.424	93.2	-16,53	4.00
CoYMnAl	Type-2	6.484	82.9	-15,96	4.72

CoYMnAl	Type-3	6.379	102.0	-14,93	-0.00
CoYMnSi	Type-1	6.093	148.0	-17,37	1.91
CoYMnSi	Type-2	6.378	99.4	-17,27	5.05
CoYMnSi	Type-3	6.250	128.1	-16,34	-0.00
CoYMnGe	Type-1	6.198	131.1	-16,55	2.90
CoYMnGe	Type-2	6.456	93.6	-16,49	5.08
CoYMnGe	Type-3	6.520	98.4	-15,58	0.00
CoYMnGa	Type-1	6.397	93.9	-15,73	4.00
CoYMnGa	Type-2	6.468	84.0	-15,39	4.74
CoYMnGa	Type-3	6.577	170.3	-15,67	5.25

3.2 Phonon properties

The calculated phonon dispersion of CoYXZ quaternary Heusler alloys, along Γ→X →W→L principal symmetry direction of the Brillouin zone (BZ) are displayed in Fig. 1 and 2. They present, respectively, the calculated phonon dispersion of CoYMnAl and CoYMnGa as prototype materials of the CoYXZ quaternary Heusler alloys. The unit cell of CoYXZ contains 4 atoms, which gives rise to 12 phonon branches, which contains 9 optical modes and 3 acoustic modes. It is clearly shown in Figures 1(a) and 2(a) that the type-1 structures of the compounds CoYMnAl and CoYMnGa are dynamically stable because none of the phonon modes has an imaginary frequency. Figures 1(b-c) and 2(b-c) show that the phonon calculation predict many imaginary phonon modes in type-2 and type-3 structure, the latter two structures are dynamically unstable. Starting from phonon dispersion bands, we notice that the optical branches and the acoustic branches are separated by gap. As a result, CoYMnZ (Z=Al and Ga)

Table3: The partial magnetic moments of CoYXZ (X=Fe and Mn; Z= Al, Si, Ge and Ga) Heusler alloys in type-1.

CoYXZ	$M_{Co}(\mu_B)$	$M_Y(\mu_B)$	$M_X(\mu_B)$	$M_Z(\mu_B)$
CoYFeAl	0.0005	- 0.0000	0.0001	- 0.0000
CoYFeSi	0.0002	- 0.0001	0.0007	- 0.0000
CoYFeGe	0.0003	- 0.0002	0.0017	- 0.0000
CoYFeGa	-0.0001	0.0000	-0.0004	0.0000
CoYMnAl	0.7793	- 0.1160	3.5712	- 0.0862
CoYMnSi	0.0684	- 0.0208	1.7692	- 0.0724
CoYMnGa	0.7338	- 0.1134	3.5695	- 0.0678
CoYMnGe	-0.2722	- 0.0307	2.1620	- 0.0781

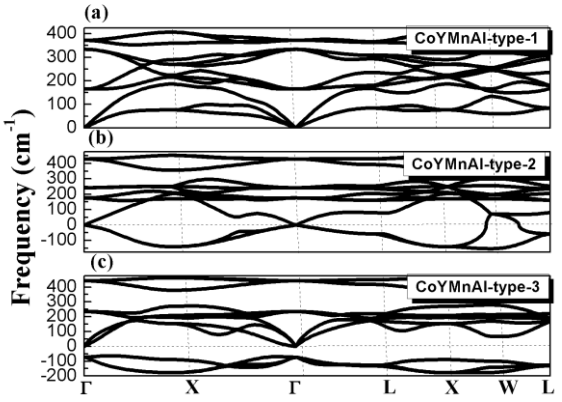

Figure 1. Calculated phonon dispersion curves for CoYMnAl Heusler alloys along lines of high symmetry in the Brillouin zone.

compounds exhibit a half-metallic behavior. At Γ point, the calculated frequencies of the optical modes are found to be 64.879, 156.288, 334.746 and 365.220 cm^{-1} for CoYMnGa-type1, 62.754, 164.392, 334.135 and 374.080 cm^{-1} for CoYMnAl-type1. To our great knowledge, there is no theoretical or experimental phonon study on the quaternary compounds that we study in this work.

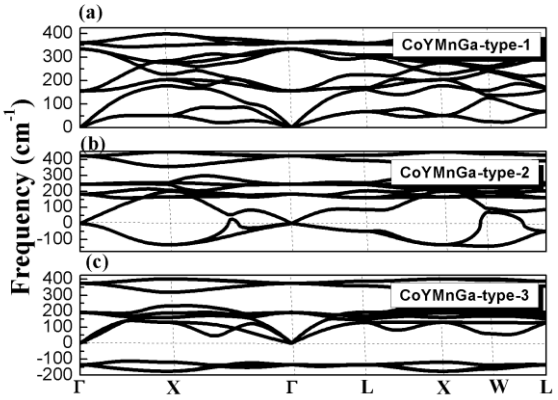

Figure 2. Calculated phonon dispersion curves for CoYMnGa Heusler alloys along lines of high symmetry in the Brillouin zone.

3.3 Magnetic properties

In what follows, our study will focus only on the type-1 structure of CoYXZ alloys. We will first calculate the magnetic properties and we will end with the electronic properties. We found four types of material family. The first type is a family of quaternary materials which has an integral magnetic moment of 4.00μ_B observed in CoYMnAl and CoYMnGa quaternary alloys. This integer

value of the magnetic moment predicts that CoYMnAl and CoYMnGa are half-metallic ferromagnetic materials. The second type of material family, formed by CoYFeZ (Z= Al, Si, Ga and Ge) alloys has a zero magnetic moment (0.00μ_B). Our result found for the material CoYFeSi is in very good agreement with the only calculation that exists [35]. The latter calculation finds zero magnetic moment in type-1 structure. The third type of material family, formed by the quaternary compounds CoYMnSi and CoYMnGe, prove to be ferromagnetic metallic with a magnetic moment of 1.91μ_B and 2.90μ_B respectively. The local magnetic moment induced by Co, Y, X (X = Mn and Fe) and Z (Z = Si, Ge, Ga and Al) atoms in the quaternary compounds are listing in table 3. It reveals that the total magnetic moment induced in the CoMnZ compounds (Z = Al, Si, Ge, Ga) is mainly due to the Mn atom. In addition, Table 3 shows that Mn atom is anti-ferromagnetically linked to t Y and Z atom in all compounds. It is also observed that Mn atom is ferromagnetically linked with Co atom except for CoYMnGe. The Co atom also provides a significant magnetic moment and the contribution of the Z atom is very small. The rest of the residual magnetic moment is due to the interstitial region.

3.4. Electronic properties

To elucidate the manifestation of the ferromagnetism, the total density of state (TDOS) is calculated in the majority spin bands (spin-up) and minority spin bands (spin-down) for the type-1 structure and at the vicinity of the Fermi level (E_F). Figures 3(a) and 4(a) shows the behavior of this density of CoYMnAl and CoYMnGa materials. It can be seen that the spin-polarized band structure exhibits a metallic behavior for the majority-state channel, while the minority spin-channel exhibits a gap at Fermi level. This result shows that CoYMnAl and CoYMnGa materials are half metallic ferromagnetic and should be suitable materials for spintronic devices. In order to analyze the contribution of different atoms and states to the valence and conduction bands, partial densities of states (PDOS) have been calculated. Figures 3(b) and 4(b) show that the upper part of the valence bands of the quaternary compounds CoYMnAl and CoYMnGa are entirely occupied by the Co and Mn states in the majority spin bands and minority spin bands, with a small contribution of the Y states and even less with the Z states. The aforementioned four graphs also show that the conduction band can be divided into two regions, the lower conduction band region within E_F to 1.5eV range and the upper conduction band region from 1.5eV to 3eV for the CoYMnAl and CoYMnGa.

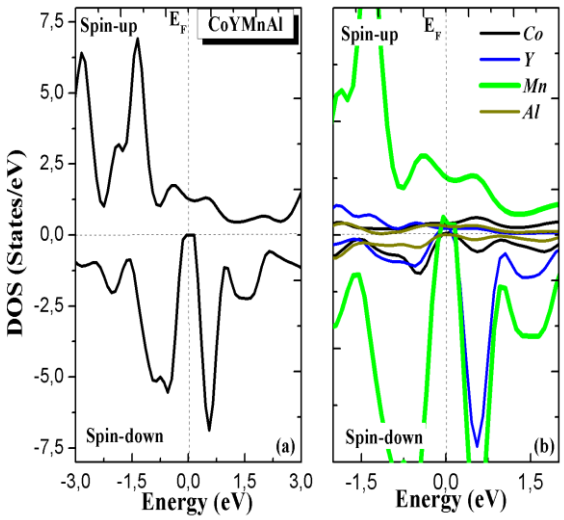

Figure 3. Calculated (a) Total and (b) Partial density of state for CoYMnAl in type-1. The Fermi level (E_F) is set to 0 eV and indicated by the vertical dashed lines.

The lower conduction band for spin-down is mainly contributed by Mn states, with a small contribution of the Co states. The upper part of the conduction band in its majority spin configuration and in its minority spin configuration shows the same contribution of all atoms states. Ferromagnetism, in CoYFeZ (Z = Al) and CoYMnZ (Z = Si, Ga and Al) emerges fundamentally from the coupling between the Co states and the Mn states.

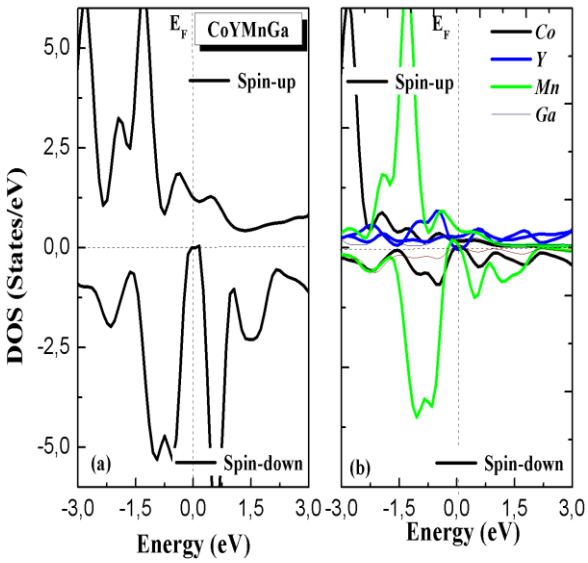

Figure 4. Calculated (a) Total and (b) Partial density of state for CoYMnGa in type-1. The Fermi level (E_F) is set to 0 eV and indicated by the vertical dashed lines.

4. Conclusion

we have performed a first principles calculation method based on density functional theory (DFT) calculation in order to study new quaternary Heusler alloys, where X (X = Fe and Mn) are transition elements belonging to the block d. The element Z (Z = Al, Si, Ge, Ga) is an element of the main group belonging to the block s or the block p. We studied the structural stability, the electronic and magnetic properties of these materials. We have explored structure of these CoYXZ materials in three different atomic arrangements (type-1, type-2 and type-3). The structural stability of these compounds was studied from the calculation of their cohesion energy and phonon dispersion, and we found that the type-1 structure is the most stable structure. From our study, the CoYMnGa and CoYMnAl quaternary compound proves to be a half-metal ferromagnetic with a total magnetic moment of 4μB. While the quaternary compounds, CoYFeZ (Z=Al, Si, Ge and Ga) seem to be not ferromagnetic, with zero moment magnetic (0.00μB). The CoYMnSi and CoYMnGe quaternary compound are found ferromagnetic with magnetic moment of 1.91μB, 2.90μB respectively. It is also divulged that the character of the half-metallicity in these compounds is closely allied to the arrangement of the transition atoms in these Heusler alloys. The magnetization of CoYMnZ (Z= Al, Si, Ga, Ge) compounds mainly comes from Mn and Co atoms. These theoretical results make these new quaternary alloys, CoYMnAl and CoYMnGa, as very promising materials for spintronic technology.

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