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Magnetic investigation of the rhodium based full-heusler material: ab initio Method

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RESUME

In recent years, heusler alloys have attracted extensive attention because of their usefulness in spintronic devices. In this paper, the structural, electronic, and magnetic properties of full heusler alloys Rh2MnZn have been studied by using the FPLAPW method based on density functional theory DFT. Calculations have been done by GGA. The investigations on the structural properties of the alloy showed that the rh2mnzn alloy had a stable structure. The results of gga calculation on electronic properties of rh2mnzn alloy show that the Rh2MnZn alloy had metallic nature due to overlapping between conduction and valance band at fermi level for both spin directions. By studying the magnetic properties, we found that the Rh2MnZn alloy were ferromagnetic materials. We showed that the compound Rh2MnZn has a technological potential for spintronics.

1. Introduction :

Magnetic materials underpin modern technologies, ranging from data storage to energy conversion to contactless sensing. However, the development of a new high-performance magnet is a long and often unpredictable process, and only about two dozen magnets are featured in mainstream applications. Full-Heusler which exhibit metallic character, the magnetic interaction is usually based on the m-J paradigm, where localized magnetic moments, m-J paramagnetically coupled through the exchange interaction, J. Only a few elements in the periodic table can provide localized moments in the solid state, namely, 3d transition metals, 4f rare earths, and some 4d ions. These materials have attracted great attentions due to their potential applications in spintronic devices, such as magnetic sensors, tunnel junctions, and giant magneto-resistance (GMR) [1, 2].

Heusler alloys are attractive because of their technical applications (in spin-injection devices [3], spin-filters [4], tunnel junctions [5], or GMR devices [6,7], their relatively high Curie temperature compared to other compounds, and their crystal structure similar to conventional semiconductors (zinc-blende and rock-salt types) [8–10]. In order to stabilise Heusler alloys practically, they should be grown on suitable substrates. Because Heusler alloys consist of 4 FCC sublattice, conventional semiconductors with zinc-blende structure (including 2 FCC sublattice) can be used as the substrate. The mismatch between thinfilm (Heusler alloys) and the substrate (semiconductors) should be as small as possible to keep the HM character of Heusler alloys in the growth process. Therefore, the lattice constant of the semiconductors must be chosen close to that of the Heusler alloys.

Heusler compounds generally take a cubic crystal structure with a 2:1:1 stoichiometry (X_2YZ) in which X and Y mainly are transition metals and Z is a main group element. X_2YZ Heusler compounds can be characterised with two different types: (1) the cubic L21 structure with a space group *Fm*.3*m* with prototype of AlCu2Mn (Fig. 1) in which X, Y, and Z atoms are placed on the Wyckoff positions 8*c* (1/4, 1/4, 1/4), 4*a* (zero, zero, 0), and 4*b* (1/2, 1/2, 1/2), respectively. The second type is the CuHg2Ti-type structure with a space group *F* .43*m* in which X atoms occupy the nonequivalent 4*a* (0, 0, 0) and 4*c* (1/4, 1/4, 1/4) positions, while Y and Z atoms are located at 4*b* (1/2, 1/2, 1/2) and 4d (3/4, 3/4, 3/4) positions, respectively [11]. In this structure, X atoms are denoted as X (1) and X (2).

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The first part of this work consists in determining the structure and the most stable magnetic phase, a study of the structural and magnetic stability was based on the procedure of the adjustment on the equation of Birch- Murnaghan [12]. The second part includes the study of the electronic properties. Finally, we study the magnetic properties of this compound: Rh2MnZn

2. Computational method :

The calculations were performed using the full-potential linearised augmented plane-wave (FP-LAPW) method within density functional theory (DFT) as implemented in the Wien2k package [13]. The exchange correlation potential (*V*XC) within the local density approximation (LDA) is calculated using the scheme of Ceperley–Alder as parametrised by Perdew–Zunger [14] and within the generalised gradient approximation (GGA) using the scheme of Perdew–Burke–Ernzerhof (PBE-GGA) [15]. In this method, the crystal is divided into nonoverlapping muffin-tin (MT) spheres surrounding the atomic sites and the interstitial regions among MT spheres. The wave functions are expanded terms of spherical harmonic functions inside MT spheres and in Fourier series in the interstitial region. The MT sphere radius for all atoms was chosen as two a.u. The potential function and charge density inside the MT spheres were expanded up to *l*max =10 and the largest vector in Fourier expansion of the charge density was *G*max = 12 (a.u.) $^{-1}$. The maximum value of the reciprocal lattice vector in the plane-wave expansion in the interstitial region (*K*max*)* was determined to be equal to 8/*R*MT, where *R*MT is the smallest MT sphere radius. The separation energy of the valence and the core electrons was chosen as −6 Ry. A mesh of 84 special *k*-points was made in the irreducible wedge of the Brillouin zone (Fig. 2). Self-consistency was achieved by setting the convergence of the charge smaller than 10^{-5} e/ (a.u.) ^{3}.

3. Results and discussion :

3.1. Structural properties :

In the first, The purpose of our study is to determine the most stable phase of the Rh2MnZn Full-Heusler alloy and for this we performed calculations of the structural, electronic, magnetic, elastic and thermodynamic properties of this compound, using the code WIEN2k [1]. The WIEN2k code algorithm is based on the DFT density functional theory [16], which is a direct application of the FP-LAPW method [17]. Our calculations were based on the generalized gradient approximation (GGA) parameterized by Perdew, Burk and Ernzerhof [18]. The latter calculates the self-consistent solution of the Kohn and Sham equations [19], which describes the valence electron in a potential created by a periodic network.

To determine the most stable structure and the magnetic phase of the compound Rh2MnZn, we carried out structural optimizations of this type of structure, for two magnetic phases: the nonmagnetic phase (NM) and the ferromagnetic phase (FM).
The structural optimization was performed by minimizing the total energy E as a function of volume V. the optimization cycle was reproduced until the imposed convergence is obtained. The modulus of compressibility at equilibrium was evaluated by adjusting the curve of variation of energy as a function of volume on the Birtch - Murnaghan equation [12] given by:

Where $E(V)$ represents the ground state energy with a cell volume V, and V_0 the volume of the unit cell at zero pressure, B_0 and B'_0 are the compressibility modulus and its derivative, respectively.
Fig. 3 shows the total energy in its magnetic (ferromagnetic, non-magnetic) phases as a function of volume for Rh2MnZn. Table **1** shows the values obtained from the structural properties of Rh2MnZn compound. Our calculations with GGA show that the ferromagnetic phase is the most energy stable for the studied alloy.

3.2. Electronic properties :

We calculated the band structures and the total and partial electronic densities of our compound; Rh2MnZn, at its fundamental structural states for the majority and minority spins along the high symmetry directions in the first Brillouin zone, using the generalized gradient approximation (GGA-PBE).
The majority and minority spin band structures for the compound Rh2MnZn are shown in Fig.4 and the Fermi level (E_f) was indicated by a black horizontal line. To understand the electronic properties of the studied alloy, the electronic band structures are calculated along the directions of high symmetry in the first Brillouin zone, shown in this Fig.4.
In the majority and minority spins, we notice that there is overlap between the conduction and valence bands, which means that this compound has a metallic character with the GGA approximation (PBE). This results in the absence of gap in both paths (spin-up, and spin-down). We note that there is a similarity in the band structures, in the two spin states (up and down).
The state density counts the number of electronic states having a given energy. The total state density allows, for example, having access to the electronic conduction properties of a material. In addition, for each atom, a sphere of given radius is defined, inside which the electron density is projected onto spherical harmonics of type (s, p, d or f). Partial state densities are thus obtained which make it possible to determine the structure of the chemical bonds between the atoms of a crystal or a molecule. The projections of the total state density depend on the radii of the spheres on which the partial state densities are projected and therefore only give access to qualitative information [20].
The total and partial state densities of compound Rh2MnZn, obtained using the generalized gradient approximation (GGA), are illustrated in Fig. 5. The results show that the Fermi level is occupied by the d states of the Mn atom and the d states of

Rh in both the majority and minority spins. Around this level, the contribution of the states Mn-d, behaves differently, in the two directions of spin.

3.3. Magnetic properties :

The total and partial magnetic moments calculated using GGA are summarized in the table. We note that the total magnetic moments of spin are not integer values. Thus, the Rh2MnZn alloy is not a Half Metallic material and it does not obey Slater's rule [21]: $M_{tot} = Z_T - 24$, or M_{tot} represents the total magnetic moment (in μB) per unit of formula and Z_T represents the total number of valence electrons. In addition, from its densities of states up and down, the values of the spin polarization of compound Rh_2MnZn are calculated.

In order to study the magnetic properties of the Heusler Rh2MnZn alloy, we present the spin density distributions (spin-up charge density minus spin-down charge density) of the conventional four-unit mesh in the figure. IV.5. From this figure, we can notice that the spin moments are located around the Mn atoms. In addition, blue iso-surfaces with a positive spin density of 0.065 / $A^{\circ 3}$ indicate that the Mn atoms are ferromagnetically coupled with Rh. The Mn atom has a significant spin comparing to the atoms of Rh and Zn. In detail, the rounded corners of the bumps for the Mn atoms are prominent. However, the magnetic moment of the atom of Mn is greater than that of the atom of Rh and Zn.
For this compound, there is no spin accumulated around the Rh and Zn atoms, demonstrating that the contribution to the total magnetic moments of these atoms is negligible. These results are consistent with the calculated total and atomic magnetic moments of the Rh2MnZn alloy, (see Table 2).

4. Conclusion :

The objective of this work is the theoretical study of the structural, magnetic electronic properties of the Full Heusler Rh2MnZn alloy, using the linearized augmented plane waves method at full potential (FP-LAPW) implemented in the WIEN2K code. The exchange and correlation effects are treated in the context of the generalized gradient approximation (GGA).
This type of material is much more popular than other classes of ferromagnetic alloys in magneto-electronic applications. The main results obtained indicate that this material studied in the direct phase (Cu2MnAl) shows that the ferromagnetic phase is the most stable. Our calculations confirm the possibility of synthesizing this material experimentally. For the electronic properties, the band structures, the densities of the partial and total states were calculated. The application of the approximation (GGA with spin) shows that our compound is a ferromagnetic metal. The band structures in the two spin channels (up and down), at equilibrium state, indicate the metallic character, represented by the overlapping of the bands at the Fermi level. The densities of total and partial states show that the Fermi level is occupied by the *d* states of the Mn atom and the *d* states of the Rh atom in both the majority and minority spins. Densities in the valence band below Fermi level are mainly due to hybridizations of the orbitals of Mn atoms with Rh-*d*. Magnetic properties: total magnetic moments of spin are not whole values. Therefore, the alloy is not an HM material and does not obey the Heusler rule [22]. In addition, the spin polarizations of the compounds are 57.8%.

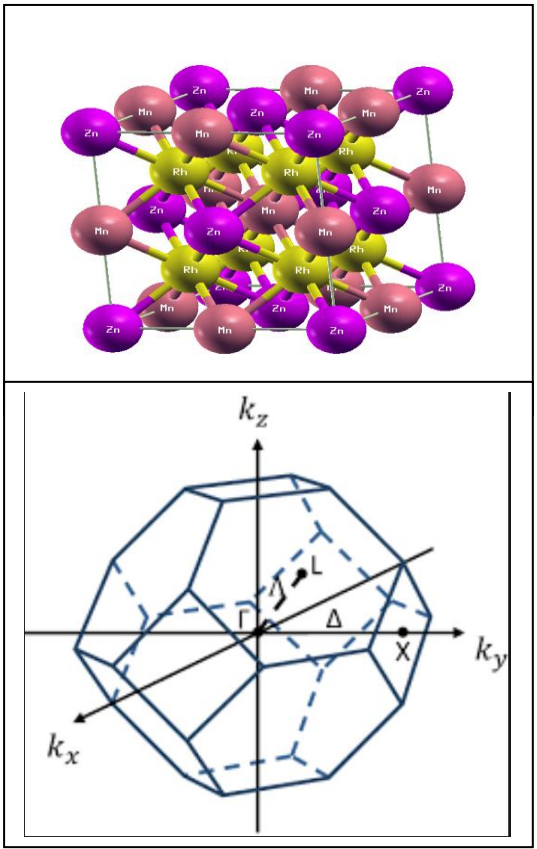


Fig. 1 : Maille conventionnelle : la structure Full-Heusler ordinaire (type AlCu2Mn de composé *Rh2MnZn*

Fig. 2 Zone de Brillouin

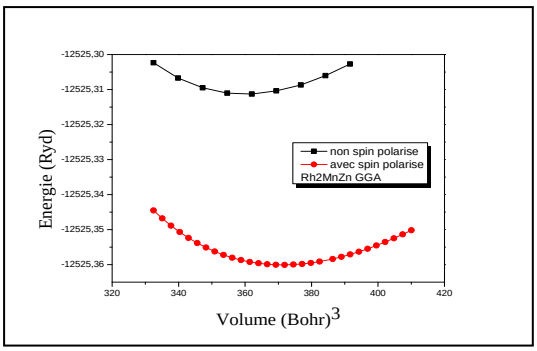


Fig. 3: Total energy of the Rh2M Zn alloy as a function of volume of the elementary cell in the two magnetic phases FM and NM.

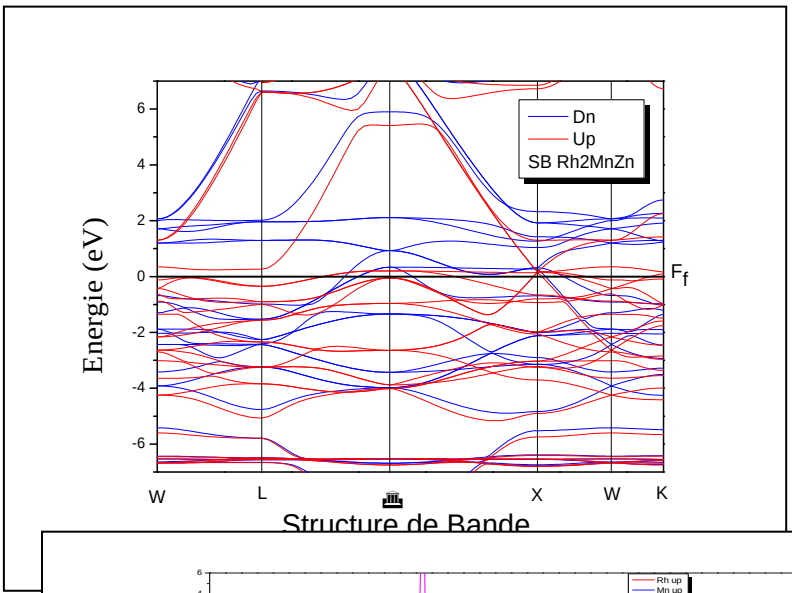
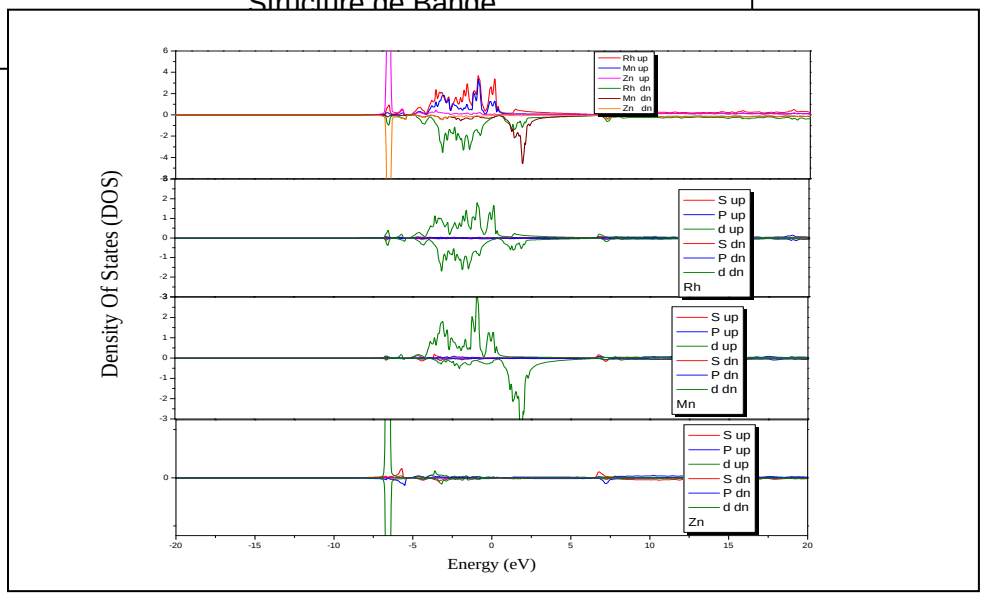


Fig.4: band the majority spins of the Rh2MnZn



Electronic structure of and minority Full-Heusler alloy

Fig. 5: Total and partial state densities of majority and minority spins of the Full-Heusler Rh2MnZn alloy

$$E(V) = E_0 + \frac{9V_0B_0}{16}\left\{\left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^3 B'_0 + \left[\left(\frac{V_0}{V}\right)^{2/3} - 1\right]^2 \left[6 - 4\left(\frac{V_0}{V}\right)^{2/3}\right]\right\} \quad (1)$$

$$P = \frac{\rho(\uparrow) - \rho(\downarrow)}{\rho(\uparrow) + \rho(\downarrow)} \quad (2)$$

Table 1: Structural properties of the Rh2MnZn alloy (cell parameter a_0, compressibility modulus B_0, its derivative B'_0, and the energy E_0).

		Results	a_0(A°)	B_0(GPa)	B'_0	V_0 (u.a.)^3	E_0(Ry)
Rh_2MnZn	GGA	Ours	5,9756	214,1809	4,7712	359,9891	-25050,622527
		Others	/	/	/	/	/
	GGA (with spin)	Ours	6 .0357	176.5512	5.3268	371.3325	-25050.720128
		Others	6.03 [23]	/	/	371.28 [23]	/

Table 2: Total and partial magnetic moments in μB and the spin polarization for the Rh2MnZn alloy

Rh_2MnZn	Results	M_{tot}	M_{int}	M_{Rh}	M_{Mn}	M_{Zn}	$\rho(\uparrow)$	$\rho(\downarrow)$	P (%)
	Ours	3.29810	0,01823	0.03524	3.22827	-0.01881	/	/	/
	Others	3.37 [23]	/	/	/	/	/	/	/

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