



Investigation of the structural, Electronic and magnetic properties of Mn_2PdSn Heusler alloy under hydrostatic pressure

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Abstract

The pressure effect on the structural, electronic and magnetic properties of Mn_2PdSn Heusler alloy was investigated by the first-principles full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). The exchange and correlation function has been chosen using generalized gradient approximation (GGA) within the parameterization of Perdew-burke-ernzerhof. The lattice constant, electronic density of state (DOS), and magnetic properties such as total magnetic moment were obtained under pressure. It was determined that the calculated lattice parameters are in good agreement with the literature. The Mn_2PdSn is stable in the Hg_2CuTi -type structure. Furthermore, we expect an extraordinary occurrence of pressure-induced metallic ferrimagnetism to half-metallic ferromagnetism transition in the cubic phase of Mn_2PdSn alloy at hydrostatic pressures of 10 GPa.

Keywords: *First principles calculations 1; Heusler alloy 2; Half-metallic 3; Pressure effects 3.*

1. Introduction

The full Heusler alloys are among a group of materials called Heusler alloys; they got this name from its first discoverer [1]. Half-metallic (HM) materials are known as materials that behave differently in the two spin bands (spin-up, spin-down), the one spin band shows metallic behaviour, while the other spin band presents semiconductor behavior [2, 3] Given this feature, these materials are promising in various fields, in particular spintronics applications [4,5,6]. Ferromagnetic materials display diverse electronic properties in the spin-up and dn bands, with metallic properties in one spin band and insulator or semiconductor properties in another, thus leading to 100% spin polarization at the Fermi [7,8,9]. Heusler alloys attracted the attention of the magnetism community the first time when F. Heusler et al. illustrated the

ferromagnetism of the Cu_2MnAl even though no one of its constituents was the ferromagnetic nature [1]. Systematic theoretical work was carried out in this study to see if the standard site preference rule applies to Mn_2 -based Heusler alloys. The competition between the XA and $L2_1$ type structures of Mn_2PdSn Heusler alloy

has been investigated by First-principle calculations. In this paper, we study the structural, electronic and magnetic properties of Mn₂PdSn, our study will also include the pressure effect on the structural electronic magnetic moment and half-metallic behavior of the alloys under study.

2. Materials and Methods

The electronic structure calculations of Mn₂PdSn are performed by the density functional theory (DFT) based on all-electron

full potential linear augmented plane wave (FP-LAPW) method, as implemented in the WIEN2K code[10]. The exchange and correlation function has been chosen using generalized gradient approximation (GGA) within the parameterization of Perdew-burke-ernzerhof [11]. We take RMT K_{MAX}=8 (where RMT is the radii of the muffin-tin sphere and K_{MAX} is the largest wave vector of the basis set). The maximum value of the angular momentum l_{MAX}= 10 is taken. In the interstitial region we take G_{MAX} = 12a.u⁻¹ for Fourier expansion. The core energy cutoff is taken as -6.0 Ry. For self-consistent convergence, the total energy was set at 10⁻⁴ Ry. The electronic configuration for Mn₂PdSn is: Mn:[Ar]4s²3d⁵;Pd:[Kr]4d¹⁰; Sn:[Kr]5s²4d¹⁰5p².

3. Result and discussions:

3.1. Structural properties:

The X₂YZ (X, Y = transition metals, Z = main group element) full-Heusler alloys have two structural configurations Cu₂MnAl prototype or Hg₂CuTi prototype [12]. In the Cu₂MnAl prototype, X atoms occupy positions 4a(0, 0, 0) and 4b(1/2, 1/2, 1/2) Y atom occupies the position 4c(1/4, 1/4, 1/4) and the Z atom occupies the d(3/4, 3/4, 3/4) position. For the Hg₂CuTi prototype, X atoms occupy (0, 0, 0) and (1/4, 1/4, 1/4) sites, Y atom enters at (1/2, 1/2, 1/2) and Z occupies (3/4, 3/4, 3/4) sites in Wyckoff coordinates [13, 14, 15]. The main distinction between these two structures is the inter-exchange of the C and B site atoms. Both structures may be indistinguishable by X-ray diffraction, and structural analysis must be performed with great care because they share the general FCC-like symmetry [16], Spin-polarized total energy was calculated as a function of volume for the compound Mn₂pdSn for both Hg₂CuTi and Cu₂MnAl structure and was fitted to the Murnaghan equation of state [17] to obtain the basic ground state properties.

$$E = E_0(V) + \frac{BV}{B'(B'-1)} \left[B \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B'} - 1 \right] \quad (1)$$

Where E₀ the minimum energy at T= 0 K, B is the bulk modulus, B' is the bulk modulus derivative and V₀ is the equilibrium volume.

Using the calculated total energy, it was possible to compare the stability of various types of structures such as Hg₂CuTi and Cu₂MnAl configurations. The result presented in figure 1 shows that the Hg₂CuTi structure has the lowest minimum energy in the energy-volume curve, making it the most stable configuration.

The number of electrons in the X and Y atoms has a considerable influence on their site selection, according to Luo and al [18] The A and C sites are preferred by elements with more electrons, whereas the B sites are preferred by those with fewer . Because the nuclear charge of X (Mn atom) is little than that of Y (Pd) so in Mn_2PdSn , the Hg_2CuTi structure will be observed. Similar results were found for Mn_2YIn ($Y=Ni, Pd$ and Pt) [19, 20] The value V_0 which corresponds to the lowest minimum energy was used to calculate the lattice parameter a_0 . For the Hg_2CuTi structure, the values were found to be 6.2313 \AA for Mn_2PdSn respectively.

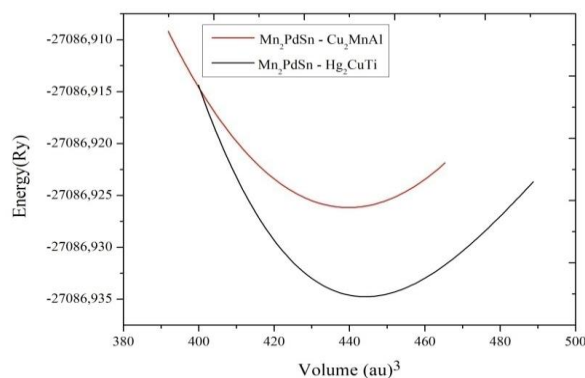


Figure 1. Calculation of the variation energy of Mn_2PdSn alloy with both Cu_2MnAl and Hg_2CuTi types structures as a function of the volume.

Table 1. Calculated lattice parameter a (\AA), bulk modulus B (GPa), its derivative pressure, the minimum energy (Ry) and the formation energy E_f (Ry) for Mn_2PdSn Heusler compound.

	$a(A^0)$	B'	$E(Ry)$	$E_f(Ry)$
$B(GPa)$				
Hg_2CuTi	6.2313	5.000	-27086.	-0.
		934796		97997
140.7873				
Mn_2PdSn	6.35 [21]			
Cu_2MnAl	6.4132	5.000		--0.
92.4660		27086.918861		96404

3.2 Electronic properties:

In order to investigate the electronic properties of the Mn_2PdSn Heusler compound, the total and partial density of states (TDOS and PDOS) for both Hg_2CuTi and Cu_2MnAl structures are calculated at the computed equilibrium lattice constants along high-symmetry directions. The TDOS and PDOS of this alloy are calculated using GGA approximation and plotted in fig 2. The positive and negative numbers correspond to the DOS of the spin-up and spin-dn states respectively, it can be observed from this figure that the DOS of This alloy at the Fermi energy in the GGA approach exhibits a metallic behaviour. Also, by paying attention to small charts focused on the Fermi energy, the metallic character of this compound is remarkably revealed. Clearly, the

predominant contribution to the band structure in the investigated energy range of -6 to 6 eV comes from the 3d transition metal Mn atoms and has a major contribution to the Fermi energy of Mn₂PdSn Heusler

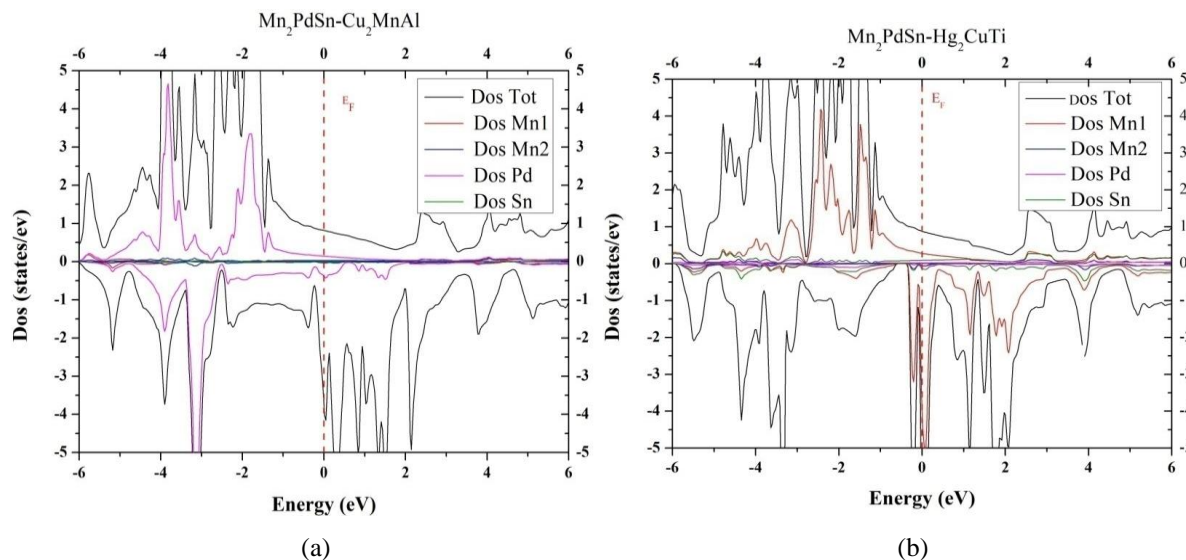


Figure 2. total and partial density of state Mn₂PdSn with (a) Cu₂MnAl and (b) Hg₂CuTi types structures

3.3 Magnetic properties:

In this part, the total and partial magnetic moment for both Hg₂CuTi and Cu₂MnAl configurations of the Mn₂PdSn Heusler compound were calculated at the equilibrium lattice parameter by GGA and listed in table 2. It can be seen that they are not integral values of the total magnetic moment for the compound which confirms that this alloy is not half-metallic. Our calculation shows that the Mn₂PdSn Heusler compound and the total magnetic moment were to be 7.56 μ_B respectively at the most stable structure with a major contribution of Mn atoms.

Table 2. Calculated total, atom-resolved, and interstitial magnetic moments (in μ_B) in the unit cell for Mn₂PdSn in their structural and magnetic ground states.

Copound	Phase	M _{tot}	M _{Mn1}	M _{Mn2}	M _y	M _{Sn}	M _{int}
Mn ₂ PdS	Hg ₂ CuTi	6.33069	2.71351	3.41314	0.20341	0.06890	0.06952
	Cu ₂ MnAl	7.56899	3.69109	3.69100	0.19998	-0.11240	0.09932

3.4. Pressure dependence on structural electronic and magnetic properties of Mn₂PdSn:

The pressure effect on the materials is a very important area since the properties of solids are directly related to inter atomic distance. Under an applied pressure the arrangement of the atoms change which lead to change the physical properties of the materials [22], The hydrostatic pressure is described by the following Murnaghan

equation if states

$$P = \frac{B_0}{B'_0} \left[\left(\frac{V_0}{V} \right)^{B'_0} - 1 \right] \quad (2)$$

Where P is the pressure, Therefore the lattice constant as a function of pressure will be:

$$a(P) = a_0 \left[1 + P \left(\frac{B'_0}{B} \right) \right]^{-\frac{1}{3B'_0}} \quad (3)$$

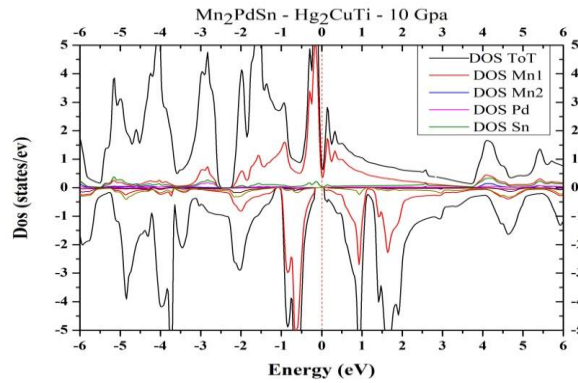


Figure 3. Total and partial density of stat under pressure of of 10 GPa for Mn_2PdSn with Hg_2CuTi type structure.

For the Hg_2CuTi structure Mn_2PdSn Heusler alloy, the total magnetic moment decrease by applying pressure and has an integer magnetic moment with a value of 4.00 μ_B for a pressure of 10 GPa which means that the compound has a half-metallic character. The effect of the pressure can be better understood with the electronic density of the state. The total and partial density of the state at a pressure of the transition from metallic to the half-metallic character (10 GPa) are presented in figure 4. The TDOS depicts that the majority spin states are metallic, whereas the minority spin states show the existence of a gap. For the Hg_2CuTi structure, Mn_2PdSn Heusler alloy behaves in metallic nature for the majority spin and semiconductor in the minority spin which confirms the half-metallic character at a pressure of 10 GPa. Also, the pressure has no influence on the Mn_2PdSn compound for the Cu_2MnAl structure.

Table 3. Variation of total magnetic moment under pressure of Mn_2PdSn for both Hg_2CuTi and Cu_2MnAl structure.

	P(GPa)	Structure	
		Hg_2CuTi	Cu_2MnAl
Mn_2PdSn	10	4.00	6.92
	20	3.97	6.50
	30	3.95	6.06
	40	3.95	5.41
	50	3.92	5.12

4. Conclusion

The structural, electronic and magnetic properties of Mn_2PdSn Heusler compound and for both Hg_2CuTi and Cu_2MnAl structure were studied by density functional calculations at zero as well as at elevated pressure. The GGA-obtained lattice parameters are in good agreement with other theoretical and experimental values. The obtained results show that the alloy behave as metal at zero pressure. The half-metallicity is observed for Mn_2PdSn at 10 GPa for Hg_2CuTi structure, with a magnetic moment of $4.00 \mu_B$.

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