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Analysis of the Structural, Electronic and Magnetic Properties of Pd_2FeTl

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Highlights

- In this study, we examine the electrical and magnetic properties of the Pd_2FeTl Heusler compound.
- The obtained results have been compared with available data in the literature.
- New data was added for Pd_2FeTl compound, and the results were reported in this paper.

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Abstract

The electronic, magnetic and structural properties of Pd_2FeTl compound were investigated in this study. The Vienna Simulation Package program was used to perform calculations, based on DFT and Generalized Gradient Approximation. The lattice parameter of $6.360A^0$ and its magnetic moment value of $3.063\mu_B$/f.u. are calculated. The values for the magnetic moment and lattice parameter were found to be in conformity with those in the literature. As electronic properties and band structures were calculated, also the density of state curves compatible with the band structures were drawn. There is no band gap between the energy bands in terms of Pd_2FeTl compound and according to the calculations, this compound has a metallic structure.

1. INTRODUCTION

Heusler compounds are the ternary compounds and Heusler type compounds were found by Friedrich Heusler with the addition of the 3rd group to CuMn compounds in 1903. It has been discovered that these compounds transform into a ferromagnetic material [1,2]. The three types of Heusler compounds are as follows: half-Heusler, full-Heusler and quaternary-Heusler compounds [3]. Half-Heusler compounds have the typical formula XYZ and a crystal structure of $C1_b$ (No:216) [4-6]. The typical formula of full-Heusler compounds is X_2YZ and the crystal structure is $L2_1$ (No:225) [7]. The usual formula for quaternary-Heusler compound is XX'YZ and they are characterized by the LiMgPdSn-type crystal form [8,9].

Half-Heusler compounds with XYZ formulas have a stoichiometric composition of 1:1:1 and are composed of three nested fcc sublattices [8]. They belong to the F-43m space group. The full Heusler compounds with X_2YZ formulas have a stoichiometric composition of 2:1:1 belonging to the space group Fm-3m [10]. The the quaternary-Heusler compounds with the XX'YZ formulas are in the 1:1:1:1 belonging to the space group F-43m [10]. X and Y are different transition metals in Full-Heusler compounds, while Z is a non-magnetic group of IIIA element. X and X' elements are transition metals in quaternary-Heusler compounds, while Z is a periodic table III-V group element [11].

The most distinctive characteristic of Heusler type compounds is that the ferromagnetic properties can change when the elements making up the compounds come together. These compounds, having ferromagnetic properties, manifest metal or semi-metallic properties. Having an important place in spintronic [12-14] and thermodynamic applications Heusler compounds. The compounds are distinctive for

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their ferromagnetic semi-metal behavior in addition to their shape and magnetic properties. Spintronic systems, magnetic memories, magnetic sensors, tunneling, and magnetic resistance applications are primarily encompassed in the fields of application of Heusler compounds.

As a result, Heusler compounds have been the subject of lots of research in recent years and there are several publications on Heusler compounds in the literature [15-17]. However, no extensive research on the characteristics of magnetism and electronics of the Pd_2FeTl compound has been undertaken so far. In his doctoral thesis, M. Gilleben only examined the lattice constant and total magnetic moment values [18]. According to the calculation results of this study, it was observed that the lattice constant and magnetic moment values were consistent with the current values known from the literature. There was no comparison was performed due to the absence of any studies related to the bulk modulus given in the Table 1. Furthermore, in the present study, band structures, DOS structures and magnetic moment values for Pd_2FeTl compound have been highlighted. The results obtained have been presented.

2. CALCULATION METHODS

Typically, exchange-correlation functionals can be solved in many ways, including the Generalized Gradient approach and LDA approaches (LDA, GGA, LSDA, mBJ) . It can be said that the simplest DFT approach is LDA or LSDA. This approach acknowledges that the load intensity of a molecular system changes very slowly. LSDA calculations are not enough to define the magnetic properties in some structures. LDA is based on the intrinsic nature of the exchange-correlation intensity distribution which does not change very fast. LDA is only dependent on local intensity while GGA also includes the intensity gradient. Despite being the simple, LDA approach may bring out quite favorable outcomes, even in realistic systems. In a more complicated approach, GGA considers spatial intensity changes as well. GGA approach may be more effective in giving better outcomes in the systems with lower binding energy and a greater lattice constant compared to LDA. Moreover, LDA approach is not good enough in the systems with spin polarization while the magnetization can be achieved to be close to the experiment through GGA approach. mBJ potential may result in better outcomes, when it is employed to examine electronic and magnetic properties, in the structures provided with a bandwidth. As better outcomes have been achieved in the calculations performed for the Pd_2FeTl compound through GGA approach, exchange and correlation effects were evaluated based on the Generalized Gradient Approach in Density Functional Theory.

Exchange and correlation effects are addressed in traditional Density Functional Theory (DFT) using Local Density Approximation (LDA) [19] or Generalized Gradient Approximation (GGA) [20,21]. For exchange correlation energy, the Perdew-Burke-Ernzerholf (PBE), GGA technique was utilized which is one of most commonly used method in quantum chemistry [22-28]. The magnetic and structural characteristics of the palladium-based Pd_2FeTl compound were first investigated using principled approaches with the Vienna Ab-initio Simulation Package (VASP, Mede-A) program [29]. The shear kinetic energy value was determined as 500 eV for the plane wave base set used in the expansion of wave functions.

Vienna Ab initio Simulation Package (VASP) program is a licensed and registered computer program configured by Mike Payne [30]. This program is capable of ab-initio generating molecular dynamics and quantum mechanical simulations. By using this, pseudopotentials, plane wave sets, PAW method, and projective coupled-wave structures within the context of intensity functional theory. Furthermore, through the VASP program, basic properties such as magnetic properties, dynamic properties, structural properties, optical properties, mechanical properties, atomic forces, static dielectric tensors can be calculated successfully.

3. THE RESEARCH FINDINGS AND DISCUSSION

The Pd_2FeTl compound was examined in the phase of $L2_1$. Figure 1 shows the crystal structure of the Pd_2FeTl Heusler compound.

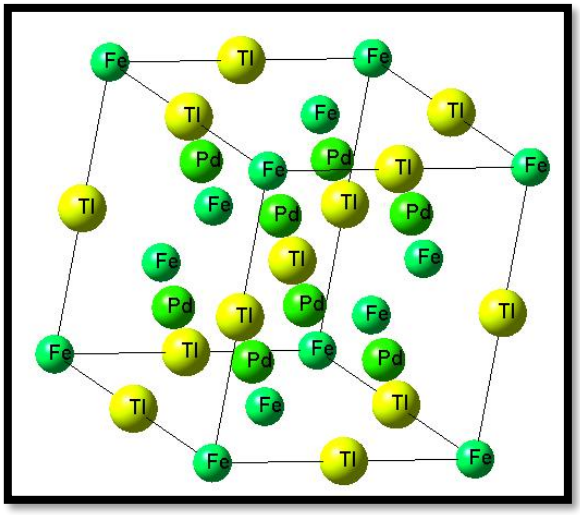

Figure 1. *The Pd_2FeTl full Heusler compound's structural optimization*

The lattice parameter, magnetic moment values and bulk modulus values of the Pd_2FeTl compound are specified in Table 1. There is one study to compare lattice parameter and magnetic moment value [18]. When the lattice constant value obtained was compared with the literature, for the Pd_2FeTl compound, the lattice constant value was determined by a difference of approximately % -1,15 while the total magnetic moment value was found by a difference of approximately % -5,17 according to the dissertation conducted by Michael Gilleben in 2009 [18]. This shows the values obtained in the present study are consistent with the current values known from the literature.

Table 1. *The parameter of the lattice (a_0), the total magnetic moment (μ_B/f.u.) and the bulk modulus (B)*

Pd_2FeTl	**a_0 (Å)**	**μ (μ_B/f.u.)**	**B (GPa)**
Present work	6.360	3.063	144.443
Theory [18]	6.434	3.230	-

Important information about the crystal's electrical conductivity and magnetic characteristics can be acquired by understanding its band structure [31]. In this study, band structures and density of states graphs Pd_2FeTl compound were obtained and analyzed. The band structures of the Pd_2FeTl compound are shown in Figure 2. In Fermi energy, a low value in the conduction band and maximum value in the valence band can be seen in the current graph in Figure 2. There is no band gap between the energy bands for the Pd_2FeTl compound and the compound has a metallic structure. This characteristic is highly significant and researched in spin-pole systems. Although the spin-pole systems are magnetically sensitive, their resistivity varies with the magnetic field. The magnetic sensors [32,33] and magnetic memory are created by diversifying resistivity in a magnetic field. Heusler compounds are used to produce polarized light emitting LEDs, tunneling magnetic resistors (TMR) and spin-spin injection devices.

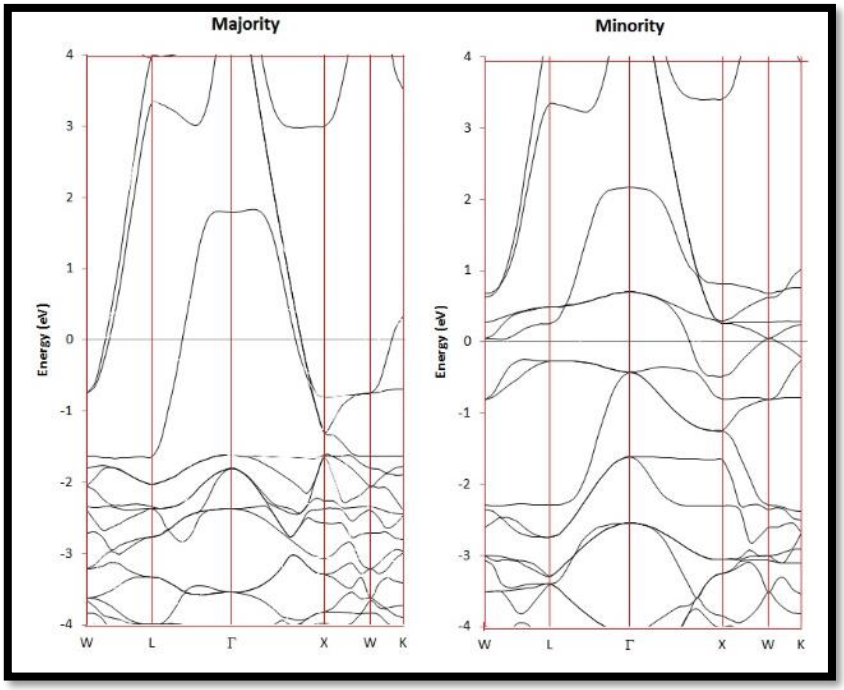

Figure 2. *The band structure of Pd_2FeTl compound*

Figures 3 present total and partial density of states curves based on spin directions for a better understanding of the contribution. Total state intensities provide information on the primary source of electron contributions to compounds. Vertical dashed lines represent Fermi energy level. Sharp peaks are dense in Fermi energy level while electrons are mostly observed in distal energy regions. As the intensity in the Fermi level reduces, the structure becomes more stable. If the state intensity in the Fermi energy level is different from zero, it means the compound has a metallic band structure. Valence and conduction bands coincide with each other at the Fermi energy level for the Pd_2FeTl compound.

The largest contribution to the sharp peaks in the spin-down and spin-up orientations is seen from the partial density of states curves in Figure 3. In there, atoms Pd and Fe for the Pd_2FeTl compound originating from the electrons in the d-orbital. As seen in the partial density of state curves, the sharp peaks around -2 eV in the spin-up state whereas -3 eV and 1 eV in the spin-down state. The knowledge are provided by electrons in the d orbitals. It can be stated that the electron contribution to the density state was negligible in the remote energy region.

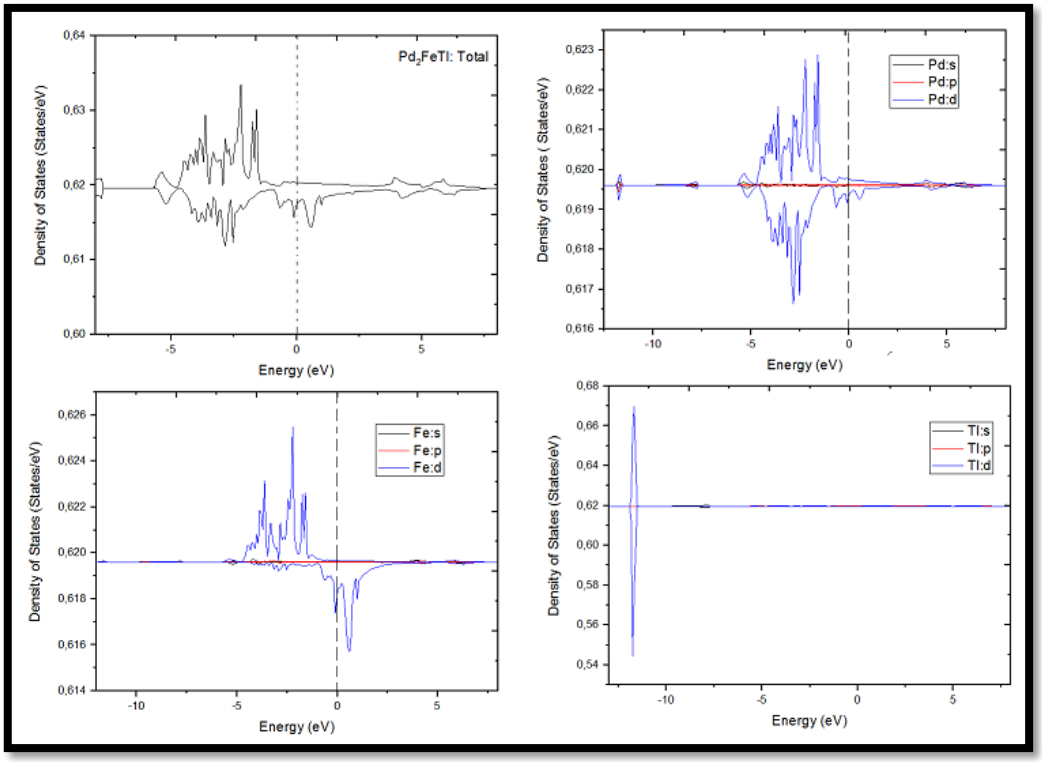

Figure 3. *The total and partial DOS of Pd_2FeTl compound*

Table 2. *The computed atomic and total magnetic moments of Pd_2FeTl compound*

μ_{Tot} (μ_B/f.u.)	μ_{Pd} (μ_B/f.u.)	μ_{Fe} (μ_B/f.u.)	μ_{Tl} (μ_B/f.u.)
3.063	0.059	3.050	-0.027

The atomic and total magnetic moment values for the Pd_2FeTl compound are shown in Table 2. According to the calculations, the total magnetic moment value of the Pd_2FeTl compound is 3.063μ_B/f.u. The magnetic moment values are 0.059 μB/f.u for Pd, 3.050 μB/f.u for Fe, and -0.027 μB/f.u for Tl. It is clearly seen in the Table 2 that the main contribution to the magnetic moment values is from the Fe atoms.

Table 3. *The values of the atomic partial magnetic moments in the Pd_2FeTl compound*

Atoms	**s**	**p**	**d**
Pd	-0.017	-0.011	0.087
Fe	0.022	0.007	3.021
Tl	0.004	-0.034	0.003

Table 3 also indicates the magnetic influence of the s,p and d orbitals on these contribution.

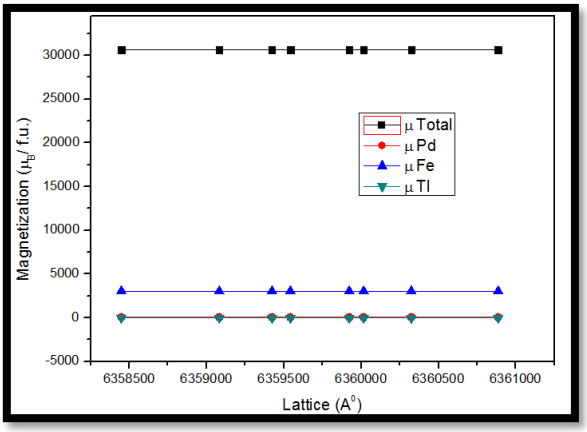

Figure 4. *The total and atomic magnetic moment of Pd_2FeTl compound*

Figure 4 shows the total and atomic magnetic moments of Pd_2FeTl as a function of lattice parameters. According to Figure 4, the total magnetic moment of Pd_2FeTl compound is calculated as 3.063μ_B/f.u.

4. RESULTS

In this research, the electronic, magnetic and structral properties of the Pd_2FeTl compound with the space group Fm-3m were examined with Density Functional Theory (DFT). The lattice parameter is 6.360 A^0 and magnetic moment is 3.063 μB/f.u. When the obtained lattice constant value was compared with the literature, for the Pd_2FeTl compound, the lattice constant value was determined by a difference of approximately % -1.15. Morover the total magnetic moment value for the Pd_2FeTl compound was found by a difference of approximately % -5.17 according to the dissertation conducted by Michael Gilleben in 2009. For the Pd_2FeTl compound, related to the Bulk modulus there are not any study in the literature. So, we have not comparison data as well. In addition to these values known in the literature, novel data has been added to the literature through the VASP program that performs calculations ab-initio and DOS structures. Thus, their magnetic properties have been intensively analyzed for the Pd_2FeTl compound. The graphs of density of states and band structures reveal that this compound has metallic properties. Such a property is highly significant for spin-pole systems. Spin-pole systems are quite susceptible to an applied magnetic field and the level of resistivity in these systems varies depending on the magnetic field. These systems are employed in the formation of magnetic memories and magnetic sensors based on the principle of resistivity variation due to the magnetic field. Consequently, it can be stated that it can be a new material for usage in spintronic and magneto-electronic devices due to the properties of the Pd_2FeTl compound.

CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

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