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Structural and Elastic Properties of Pd_2CrPb Heusler Compound

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Abstract: Electronic, structural and elastic properties of Pd_2CrPb compound were examined with Density Functional Theory (DFT). The lattice constant in state of balance and the total magnetic moment value were calculated and 6.454 A^0 and 3.678 μB f.u. values were obtained respectively. The lattice constant and total magnetic moment value obtained for Pd_2CrPb compound were compared to existing values in the literature, and the results obtained were found to be consistent with the literature results. The calculation of bulk modulus in this study is non-existent in the literature. The bulk modulus of this molecule is presented in the literature in this sense. The aim of the study is to publish the results of studies on non-existent electronic, structural and elastic properties for Pd_2CrPb compound conducted using density functional theory. The electronic band structure, total and partial density graphs for Pd_2CrPb compound were drawn. Bulk modulus (B), Shear modulus (G), B/G ratio, Young modulus (E), Poisson ratio, C_{11}, C_{12} and C_{44} values were also calculated for this compound. Pd_2CrPb compound meets Born stability principles and calculated elastic stabilities show that this compound is mechanically stable.

Keywords: Band structure, Pd_2CrPb, GGA-PBE, Density functional theory

Pd_2CrPb Heusler Bileşiğinin Yapısal ve Elastik Özellikleri

Öz: Yoğunluk Fonksiyonel Teorisi (DFT)ile Pd_2CrPb bileşiğinin elektronik, yapısal ve elastik özellikleri incelenmiştir. Denge durumundaki örgü sabiti ve toplam manyetik moment değeri hesaplanmıştır ve sırasıyla değerleri 6.454 A^0 ve 3.678 μB f.u. bulunmuştur. Pd_2CrPb bileşiği için elde edilen örgü sabiti ve toplam magnetik moment değerleri literatürde mevcut olan değerler ile karşılaştırılmış ve elde edilen sonuçların literatür sonuçlar ile uyumlu olduğu gözlemlenmiştir. Bu çalışmada yapılan bulk modülü hesaplaması literatürde mevcut değildir. Bu anlamda literature bu molekülün bulk modülü sunulmuştur. Pd_2CrPb bileşiği için literatürde mevcut olmayan elektronik, yapısal ve elastic özellikleri ile ilgili çalışmalar yoğunluk fonksiyon teorisi yardımı ile gerçekleştirilerek elde edilen sonuçların literature kazandırılması amaçlanmaktadır. Pd_2CrPb için elektronik bant yapıları, toplam ve kısmi durum yoğunluğu grafikleri çizilmiştir. Ayrıca bu bileşik için Bulk modülü (B), Shear modülü (G), B/G oranı, Young modülü, Poisson oranı, C_{11}, C_{12} ve C_{44} hesaplanmıştır. Pd_2CrPb bileşiği Born kararlık ilkelerini sağlamaktadır ve hesaplanan elastik sabitleri bu bileşiğin mekaniksel olarak kararlı olduğunu göstermiştir.

Anahtar Kelimeler: Band yapısı, Pd_2CrPb, GGA-PBE, Yoğunluk fonksiyonel teorisi

1. Introduction

When elements that form Heusler's compounds come together, it is discovered that these compounds transform ferromagnetic material, and they are an ideal material group for spintronics and magneto-electronic practices due to their interesting magnetic properties. First Heusler type compounds were discovered adding 3rd group element aluminum to CuMn alloy by Friedrich Heusler in 1903 (Heusler, 1903).

Heusler compounds crystallize in stoichiometric order, when full and semi-Heusler compounds crystallizing in the $L2_1$ and $C1_b$ structures (Offernes et al., 2008; Otto et al., 1987; Otto et al., 1987). Heusler compounds have four fcc substrings interwoven with positions (0,0,0) and (1/2,1/2,1/2) for the X atom, (1/4,1/4,1/4) for the Y atom, and (3/4,3/4,3/4) for the Z atom. Semi-Heusler compounds are made up of four interwoven substrings, three of which are ridden with X, Y, and Z atoms, while the fourth (1/2,1/2,1/2) is empty. The $C1_b$ structure is formed by changing half of the X sites in neat form from the $L2_1$ structure. Full Heusler compounds with X_2YZ formulas have a 2:1:1 stoichiometric composition and are in the Fm-3m space group (Xing et al., 2009). Quaternary Heusler compounds with XX'YZ chemical formula are in the 1:1:1:1 stoichiometric composition and in the F-43m space group (Xu et al., 2013). In full Heusler compounds, when X and Y are generally two different transition metals, Z is a non-magnetic III-VI A, i.e., sp group element. In quaternary Heusler compounds, when X, X' and Y elements are in the transition metal group, and Z elements are in the III-V group of the periodic table. LiMgPdSn structure can be shown as an example for quaternary Heusler compounds (Xu et al., 2013; Eberz at al., 1980).

Many studies have been conducted on Heusler compounds, but no comprehensive study on the electronic and elastic properties of Pd_2CrPb compound has been completed. In his doctoral thesis, M. Gilleßen (Gilleßen, 2009) only examined the lattice constant and total magnetic moment values. The VASP package program was used to examine the basic properties of the Pd_2CrPb compound, and new data were included, and the results were shared.

The band, partial and total DOS structures, as well as the electronic properties of compounds, were the focus of this research. Elastic stabilities for compounds were also calculated and with the help of obtained elastic stabilities, these compounds are determined to be mechanically stable.

2. Material and Method

All calculations for Pd_2CrPb compound were made by using the VASP (Meda-A) package program based on density functional theory. Generalized Gradient Approximation (GGA) was used by using the Perdew-Burke-Ernzerholf (PBE) diagram (Kresse and Hafner, 1993;1994; Kresse and Furthmüller, 1996; 1996; Perdew et al., 1996). The energy cutoff value was taken as 500 eV, and the Brillouin region was studied using 4x4x4 k-dots generated by the Monkhorst-Pack scheme. In this study, primarily lattice

constant, bulk modules, and total magnetic moment values within the scope of structural parameters were calculated for Pd_2CrPb compound. Shear modulus, B/G ratio, Young modulus and Poisson ratio were searched for Pd_2CrPb by obtaining elastic stables.

3. Results and Discussion

Pd_2CrPb compound is examined for the Palladium-based in the $L2_1$ phase, which has a Fm-3m space group and crystallizes in a cubic structure. Fig. 1 shows the crystal structure of the Pd_2CrPb compound. The total magnetic value and balance lattice stability were obtained. Lattice parameter and total magnetic moment values are in Table 1 with existing theoretical data. Obtained values for the compound are in good agreement with existing results.

Table 1. The lattice constant (A^0) and total magnetic moment (μB f.u)

Pd_2CrPb	a_0 (Å)	M (μb f.u.)
Present work	6.454	3.678
Theory (Gilleßen, 2009)	6.553	3.90

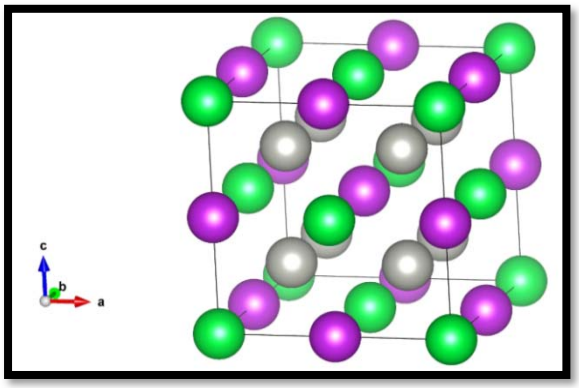

Figure 1. The structural optimization of Pd_2CrPb full Heusler Compound

Lattice parameter and total magnetic moment values are in Table 1 with existing theoretical data. Obtained values for the compound are in good agreement with existing results.

Elastic properties of a cubic crystal establish a connection with the mechanical properties of that crystal and give critical information about its stability. Flexibility stables of cubic crystal are shown as C_{ij} and are defined by C_{11}, C_{12} and C_{44} (Luan et al., 2018; Rassoulinejad-Mousavi et al., 2016). Cubic crystals have to meet Born stable principles to be mechanically stable. Born stable principles for cubic crystals are below ; (Mogulkoc, et al. 2013; Wu et al., 2007; Mouhat and Coudert 2014);

$$C_{11} > 0, C_{44} > 0, C_{11} > |C_{12}|, (C_{11} + 2C_{12}) > 0 \quad (1)$$

The mechanical stability of the Pd_2CrPb compound was analyzed in terms of the elastic stables. Table 2 shows the values found for the elastic stables, and when the obtained values are examined, it is seen that the Pd_2CrPb compound meets the Born stability principles and is mechanically. Bulk modulus (B), Shear modulus (G), B/G ratio, Young modulus (E), Poisson ratio values were also calculated for this compound and all these calculated were listed at Table3.

Table 2. The calculated elastic constants C_{ij} (C_{11}, C_{12}, and C_{44}).

C_{11} (Gpa)	C_{12} (Gpa)	C_{44} (Gpa)
139.664	126.765	69.858

Table 3. The calculated Bulk modulus (B), Shear modulus (G), B/G ratio, Young modulus (E) and Poisson ratio (ν).

Compound	B	G	B/G	E	ν
Pd_2CrPb	131.064	29.328	4.47	81.878	0.40

When the unit cell of the crystal is in the state of balance and minimal strains are applied, the Bulk modulus is obtained using the energy change. The Bulk modulus is a measure of the resistance against volume change under applied pressure.

The mechanical properties of Pd_2CrPb compound were investigated using the bulk modulus to shear modulus ratio (B/G). According to Pugh criteria, when the B/G ratio is below 1.75, the material shows brittle behavior, and when the B/G ratio is above 1.75, the material shows ductile behavior (Mouhat and Coudert, 2104; Perdew et al., 1993; Pugh, 1954).

Shear modulus is a measurement of the material's stretching under shears or resistance to lateral pressure; as a result, the shear modulus determines hardness better than isotropic compressibility modules. The Young modulus is expressed as the ratio of the tensile strain to the tensile strength, and a high Young modulus indicates that the material is hard.

The Poisson ratio is an essential property of materials that provides information about the characteristics of binding forces. When covalently bound materials have a Poisson ratio of about 0.1, electrostatically bound materials have a Poisson ratio of about 0.2. These values for Pd_2CrPb compound were calculated and are shown in Table 3. As can be seen in Table 3, the Pd_2CrPb compound has a ductile structure and an electrovalent character.

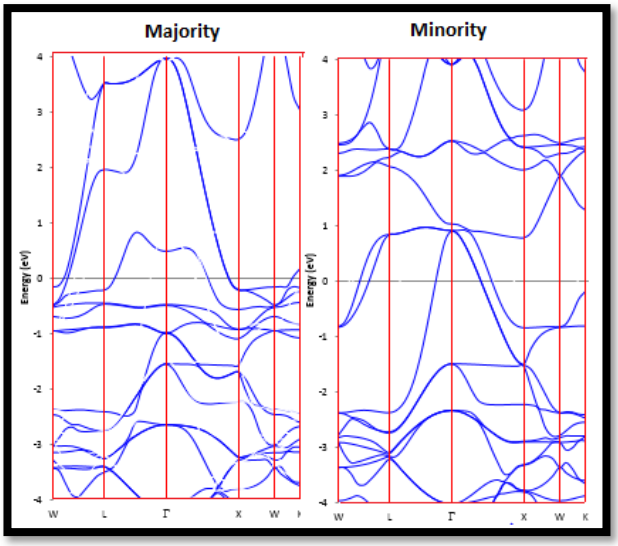

Figure 2. The band structure of Pd_2CrPb Compound

For Pd_2CrPb compound in $L2_1$ structure, spin-polarized band structures are given in Fig. 2 along high symmetry directions in the first Brilloin region. As shown in Fig.2, there is no electronic space for either the upper or lower spin, and the conductivity and valence bands are interwoven. Fig. 3 shows the total density of states in order to better analyze the electronic contribution for Pd_2CrPb compound and energy space, which does not

exist at the fermi level. This situation shows that polarized band structures exhibit metallic behavior in both spin orientations.

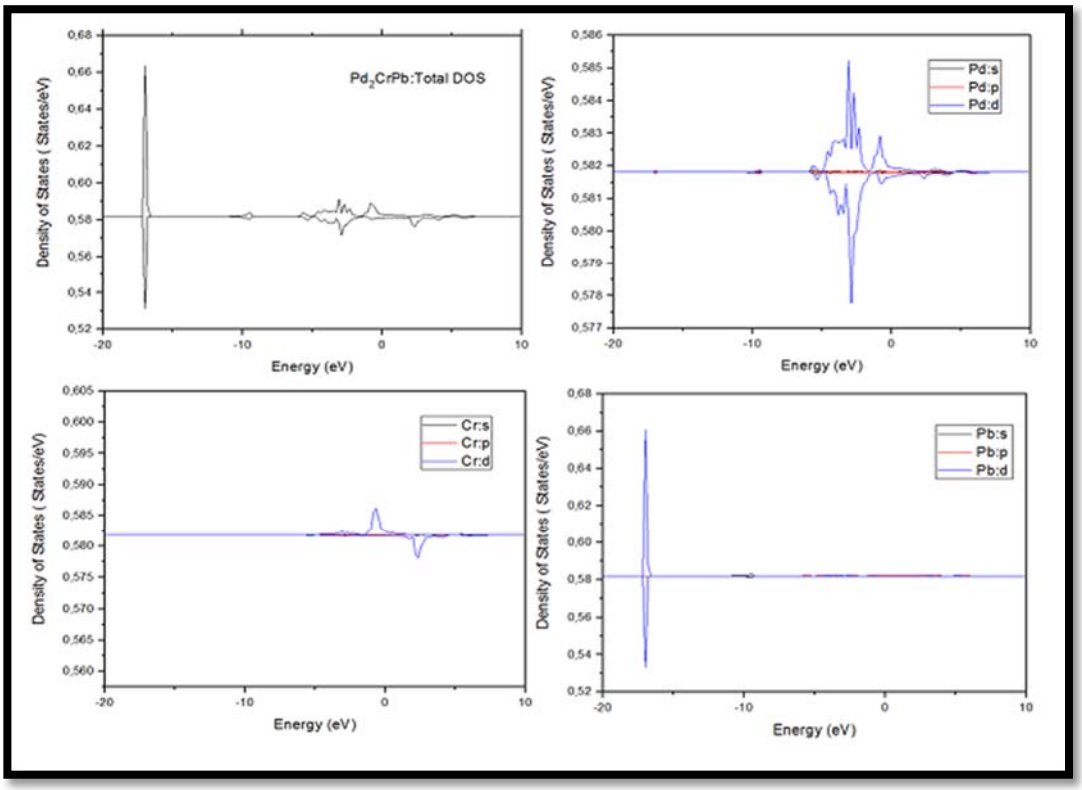

Figure 3. The total and partial DOS of Pd_2CrPb Compound

In this study, the electronic, structural, and elastic properties of Pd_2CrPb compound that is in Fm-3m space group and cubic structure were investigated using DFT theory, which is a theoretical model for Pd_2CrPb compound in Fm-3m space group and cubic structure. The compound's lattice parameter and total magnetic moment were calculated, and the results were found to be consistent with the existing values in the literature. Bulk modules of Pd_2CrPb compound were also obtained; however, no comparison of this value can be made because there is no experimental and theoretical study about this compound in the literature. The band structure, partial and total density of state diagrams for Pd_2CrPb compound were obtained, and because the Fermi level has finite energy, the compound exhibits metallic behavior. Since the obtained B/G ratio of Pd_2CrPb compound is greater than 1.75, it is understood that the material exhibits ductile behavior. Elastic properties of Pd_2CrPb compound are presented first in this study and calculated analysis of elastic stables shows that Pd_2CrPb compound is in the stable structure. Due to the properties of the Pd_2CrPb compound, it can be said that the Pd_2CrPb compound is a prospective material for magneto-electronic and spintronic practices.

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