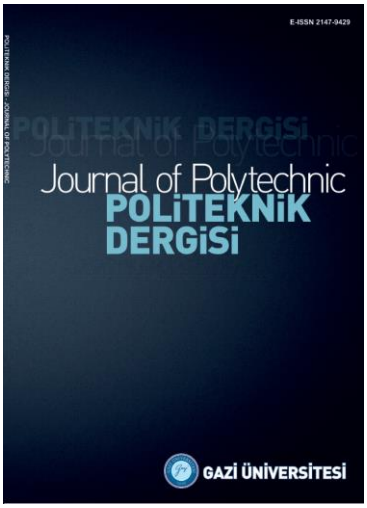

POLİTEKNİK DERGİSİ

JOURNAL of POLYTECHNIC

ISSN: 1302-0900 (PRINT), ISSN: 2147-9429 (ONLINE)
URL: http://dergipark.gov.tr/politeknik

The investigation DO_3-type Fe_3M (M=Al, Ga, Si and Ge) full-heusler alloys within first principles study

İlk prensipler ile DO_3-tipi Fe_3M (M=Al, Ga, Si ve Ge) tam heusler alaşımlarının incelenmesi

***Yazar(lar) (Author(s))**: Aytac ERKISI[1], Gokhan SURUCU[2]*

ORCID[1]: 0000-0001-7995-7590

ORCID[2]: 0000-0002-3910-8575

Bu makaleye şu şekilde atıfta bulunabilirsiniz(To cite to this article): Erkisi A. ve Surucu G., "The investigation DO_3-type Fe_3M (M=Al, Ga, Si and Ge) full-heusler alloys within first principles study", ***Politeknik Dergisi***, 21(4): 927-936, (2018).

Erişim linki (To link to this article): http://dergipark.gov.tr/politeknik/archive

DOI: **10.2339/politeknik.385443**

The Investigation DO_3-type Fe_3M (M=Al, Ga, Si and Ge) Full-Heusler Alloys Within First Principles Study

Research Article / Araştırma Makalesi

Aytac ERKISI[1*], Gokhan SURUCU[2,3,4]

[1]*Department of Physics Engineering, Hacettepe University, Beytepe, Ankara, 06800, Turkey*
[2]*Department of Electric and Energy, Ahi Evran University, Kırşehir, 40100, Turkey*
[3]*Middle East Technical University, Department of Physics, 06800, Ankara, Turkey*
[4]*Photonics Application and Research Center, Gazi University, Ankara, 06500, Turkey*

(Received : 21.08.2017 ; Accepted : 28.09.2017)

ABSTRACT

Full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys whose crystal structure is DO_3-type disordered structure which conforms to $Fm\bar{3}m$ space group, have been investigated by using Local Spin Density Approximation (LSDA) and Generalized Gradient Spin Approximation (GGSA) in the Density Functional Theory (DFT) as implemented in VASP (Vienna Ab initio Simulation Package) software. After the examination of ground states of our materials in DO_3-type structure, their full structural, mechanical properties and electronic band structures have been investigated and made comparison between LSDA and GGSA. The calculated electronic band structures and total electronic density of states (DOS) within both of two approximation show that these alloys have metallic behavior. The calculated elastic constants and estimated mechanical properties depended on these constants indicate that these alloys are stable mechanically and have anisotropic behavior.

Keywords: Full-Heusler; Ab initio calculations, elastic constant, electronic band structure.

İlk Prensipler ile DO_3-tipi Fe_3M (M=Al, Ga, Si ve Ge) Tam Heusler Alaşımlarının İncelenmesi

ÖZ

Kristal yapısı DO3-tipi düzensiz yapıda olan ve Fm$\bar{3}$m uzay grubuna uyan tam-Heusler Fe3M (M=Al, Ga, Si and Ge) alaşımları, Yoğunluk Fonksiyonel Teorisi (DFT) altında Yerel Spin Yoğunluk Yaklaşımı (LSDA) ve Genelleştirilmiş Gradient Spin Yaklaşımı (GGSA) kullanılarak VASP (Vienna Ab initio Simulation Package) yazılımı ile incelenmiştir. DO3-tipi yapıda olan malzemelerimizin taban durumlarının incelenmesinden sonra tam yapısal, mekaniksel özellikleri ve elektronik band yapıları incelenmiş ve GGSA ve LSDA arasında karşılaştırma yapılmıştır. Her iki yaklaşım içinde hesaplanan elektronik band yapıları ve toplam elektronik durum yoğunlukları (DOS) bu alaşımların metalik davranışa sahip olduklarını göstermektedir. Hesaplanan elastik sabitler ve bu elastik sabitlere bağlı olarak tahmin edilen mekaniksel özellikler bu alaşımların mekaniksel olarak kararlı ve anizotropik davanışa sahip olduklarına işaret eder.

Anahtar Kelimeler: Tam-Heusler, Ab initio hesaplamaları, elastik sabiti, elektronik band yapısı.

1. INTRODUCTION

Heusler type alloys which are ternary intermetallics, were discovered first by Friedrich Heusler in the early 20th century [1]. There is two type Heusler alloys which are called half-Heusler are given XYZ and full-Heusler alloys are given X_2YZ general formulas, respectively. Some researchers have worked on these type alloys and investigated that the composition, chemical order and magnetic properties of these alloys are related with each other [2,3]. In recent years, some scientists have shown great interest in these materials due to the diverse and attractive physical phenomena such as magnetic shape memory effect, magnetocaloric effect, magnetothermal conductivity, magnetic superelasticity, exchange bias, and half-metallic ferromagnetism exhibited by them [4-9]. Moreover, Heusler alloys can be used such as half-metallic ferromagnets, semiconductors and superconductors [10-13].

The full-Heusler alloys have a fully ordered $L2_1$ type face centered cubic structure which conform $Fm\bar{3}m$ space group at room temperature [14]. There are four interpenetrating sublattices which have face centered cubic (fcc) structures, in the unit cell of these type alloys. Atomic positions with Wyckoff notation in full-Heusler alloys are (0 0 0) for X_1, (1/2 1/2 1/2) for X_2, (1/4 1/4 1/4) for Y and (3/4 3/4 3/4) for Z atom abbreviated A, B, C and D sites, respectively. X and Y elements in compositions are usually a transition metal, Z element can be either a semiconductor or a non-magnetic metal.

When the X, Y and Z atoms are located in their original positions, this type structure of a crystal is called $L2_1$ ordered structure. The partially disordered structure is called B2-type structure which in the X_1 and X_2 atoms are

*Sorumlu yazar (Corresponding Author)
e-posta : erkisi@hacettepe.edu.tr

positioned in (0 0 0) and (1/2 1/2 1/2) atomic positions with respectively and Y and Z atoms are randomly sited. If there is the distribution of X and Y or X and Z atoms randomly, this crystal behaves DO_3-type disordered structure of full-Heusler alloys [15]. The crystal structure of Fe_3Si is ordered DO_3-type as seen in Fig.1. This alloy possesses two non-equivalent $Fe_{A,C}$ in A and C sites and Fe_B in B sites since magnetic moments of Fe atoms in these sites are different from each other. Therefore, this material sometimes referred to as $Fe_2^{AC}Fe^{B}Si$. This is similar to fully ordered full-Heusler alloy in ordered $L2_1$ crystal structure [16]. Ordered crystal structures show considerable mechanical, electrical, magnetic and physical properties. The type and degree of the atomic order are affected on the electronic band structure of Heusler alloys. A partially disordered crystal structure can lead to seriously changing in their electronic band structure, magnetic and transport properties [17-20]. Therefore, this type of alloys is much important for the technological applications.

In this view, we have examined full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3-type structure and also made comparison between two approximation which are LSDA and GGSA. The computational details are given in the next section. The examined and calculated some structural, mechanical properties and also electronic band structure with density of states (DOS) of these alloys are discussed in the third section. Finally, we have concluded our calculations in the last section. To the extend we know, there is no detailed study especially for the Fe_3Ga and Fe_3Ge alloys.

2. COMPUTATIONAL DETAILS

In this work, the calculations have been made with VASP (Vienna Ab initio Simulation Package) [21,22] package and utilized linear augmented-plane-wave basis set and psuedopotential approximation. We have used Projected Augmented Wave (PAW) [23,24] with the Perdew-Zunger correlation [25] type pseudopotentials for all atoms in the framework of Local Spin Density Approximation (LSDA) and Perdew, Burke and Ernzerhof (PBE) [26] type pseudopotentials in the framework of Generalized-Gradient Spin Approximation (GGSA) within Density Functional Theory (DFT) [27,28], to approximate exchange-correlation potential. The crystal structure of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys has been examined in $Fm\bar{3}m$ space group. 14×14×14 k-point mesh has been automatically generated and used to irreducible Brillouin zone yielding 280 k-points centered at Γ-point. Brillouin-zone integrations have been performed following the convention of Monkhorst-Pack [29] scheme. The kinetic energy cut-off value has been took 1100 eV for wave-functions in plane wave basis sets expansion of eigenfunctions. The crystal structure of DO_3-type full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in cubic ($Fm\bar{3}m$) phase with 4-atom primitive cell is presented in Fig.1. The ionic relaxation process has been went on until the forces on ions are less than 10^{-8} eV/Å. The lattice parameters and atomic positions of atoms in the primitive cell of the crystal have been optimized by minimizing of the forces and the pressure on these systems.

3. RESULTS AND DISCUSSION

Firstly, it is determined the primitive cells of Fe_3M (M=Al, Ga, Si and Ge) full-Heusler alloys in DO_3 structure which are modeled by four atoms and whose three dimensional (3D) crystallographic representation is shown in Fig.1.

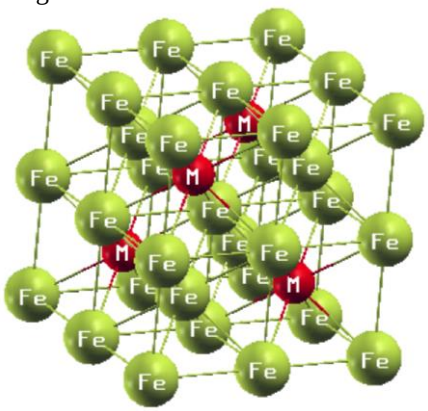

Fig. 1. The three dimensional (3D) crystallographic representation Fe_3M (M=Al, Ga, Si and Ge) full-Heusler alloys in DO_3-type structure with $Fm\bar{3}m$ space group.

Fe_3M (M=Al, Ga, Si and Ge) alloys can be viewed as full-Heusler alloys in DO_3-type structure with $Fm\bar{3}m$ space group as seen in Fig. 1. The A, B and C sites have been occupied by Fe atoms and the D sites have been occupied by M atoms in this crystal system. These alloys have been optimized by using two different type approximation which are LSDA and GGSA. In the next step, the calculated energy and volume datas for our materials have been plotted as a graphic by fitting to Vinet [30] equation of state. After this process; the structural, mechanical properties and also electronic band structures with density of states (DOS) of these sytems have been calculated by using LSDA and GGSA.

3.1. The Calculated structural properties by using GGSA and LSDA approximation

The calculated structural properties of Fe_3M (M=Al, Ga, Si and Ge) full-Heusler alloys by using LSDA and GGSA, have been presented in this section. To examine structural stability of these alloys, the cohesive energies (E_{coh}) [31,32] of them which is given in Eq.1, have been calculated. The cohesive energies of any crystal which has the chemical formula A_xB_y, can be calculated by the following,

$$E_{coh} = E_{tot} - (xE_A + yE_B) \quad (1)$$

where, E_{tot} is the total energy of the unit cell of the crystal. E_A and E_B are the energies of the isolated A and

B atoms as seen in Eq. 1. The calculated cohesive energies of these alloys by using two different type approximation have been presented in Table 1. The calculated cohesive energies within both LSDA and GGSA show that, our materials are structurally stable and synthesizable due to the negative values.

After the optimization processes of Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA and LSDA, energy-volume graphs are plotted by fitting to Vinet equation of state [30] which is given by

$$E(V) = E_0 + \frac{9BV_0}{\xi^2}[1 + \{\xi(1-x) - 1\}\exp\{\xi(1-x)\}] \quad (2)$$

where E_0 and V_0 are the ground state energy and volume, respectively, $x = (V/V_0)^{1/3}$ and $\xi = (3/2)(B' - 1)$, B is the bulk modulus and B' is its pressure derivative. These fitted curves and also calculated some structural parameters of our alloys within GGSA and LSDA are presented in Fig. 2 and in Table 2 with respectively. It has been obtained a well-converged ground state for these alloys with both of GGSA and LSDA due to the asymptotic standard errors in fitting the Vinet equation of state are less than about 1%

The calculated some structural parameters of Fe_3Si alloy in DO_3 structure by using GGSA (a = 5.608 Å, B = 204.79 GPa) and LSDA (a = 5.462 Å, B = 268.93 GPa), are very close to the experimental (a = 5.646 Å [16], B = 187 GPa [33]) and theoretical results (a = 5.630 Å [34], B = 199 GPa [34] within GGA and a = 5.490 Å [34], B = 242 GPa [34] within LDA). The obtained lattice parameter (a) and bulk modulus (B) of this alloy within GGSA are different % 0.67 and % 9.5 from experimental results and % 0.39 and % 2.9 from theoretical results, respectively and also within LSDA are different % 3.3 and % 43 from experimental results and % 0.51 and % 11 from theoretical results, respectively. Similarly, the calculated lattice parameters of Fe_3Al alloy in DO_3 structure within GGSA (a = 5.748 Å) and LSDA (a = 5.560 Å), are very close to the experimental (a = 5.789 Å [35]) and theoretical results (a = 5.761 Å [35] with GGA and a = 5.718 Å [36] with LDA). The obtained lattice parameter (a) of this alloy within GGSA is different % 0.7 from experimental result and % 0.22 from theoretical result, respectively and also within LSDA is different % 3.9 from experimental results and % 2.7 from theoretical result, respectively. Also calculated bulk modulus by

Table 1. The calculated cohesive energies of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA and LSDA.

Material	GGSA E_{coh} (eV)	LSDA E_{coh} (eV)
Fe_3Al	-27.711	-31.170
Fe_3Ga	-26.521	-30.268
Fe_3Si	-29.897	-33.778
Fe_3Ge	-28.114	-32.029

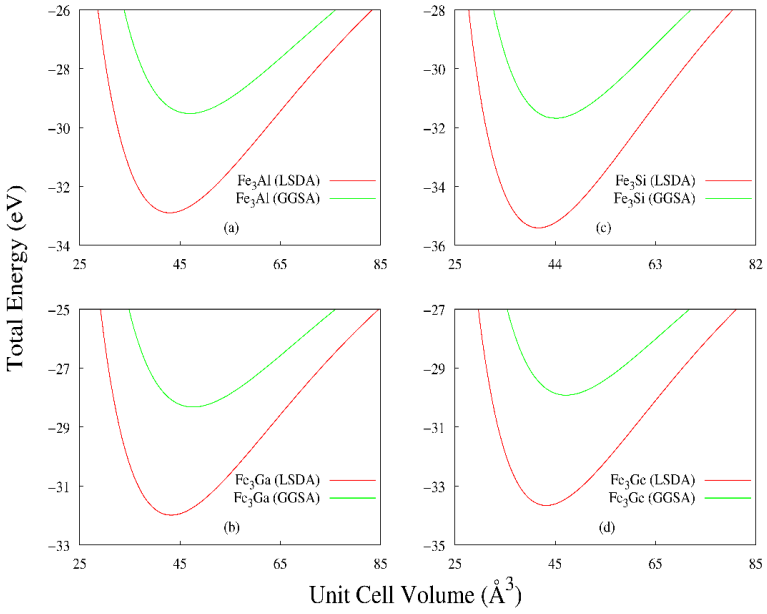

Fig. 2. Total energies as a function of volume of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA and LSDA.

using GGA (B=160.99 GPa) is very close to theoretical result (B = 167 GPa [35]). The calculated lattice parameter of Fe_3Ga alloy in DO_3 structure within GGSA (a = 5.772 Å) are very close to the other theoretical result (a = 5.761 Å [37] within GGA) too. It is obviously seen that, the calculations of structural parameters for Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA seems more accurate than LSDA.

3.2. The calculated magnetic moments within GGSA and LSDA

It can be seen as an fcc Bravais lattice with a basis consisting of four atoms, *A, B, C* and *D*, associated with each lattice point for the ordered Fe_3M (M=Al, Ga, Si and Ge) alloys crystallized in the DO_3 structure. For these alloys, Fe atoms which are equivalent, are located at the A (Fe_A) and C (Fe_C) sites. Also the B-sublattice is located with iron atoms (Fe_B) whereas M atoms (M=Al, Ga, Si and Ge) occupy the D sites. The centre of the cube is occupied with Fe_B atom whereas four Fe_A and four Fe_C atoms are located at the corners of cube. So, Fe_B is eightfold coordinated with the other Fe atoms, and the point symmetry is cubic. Therefore, the calculated partial magnetic moment with of Fe_A and Fe_C are equal with each other and the partial magnetic moment of Fe_B is different from them. Moreover, the partial magnetic moments we compute are compatible with the experimental work (for Fe_3Al and Fe_3Si alloys) [36] and also the obtained magnetic moments within GGSA is more closer than within LSDA as seen in Table 3.

3.3. The calculated elastic constants and estimated mechanical properties

Elastic constants of a crystal which can be calculated in theoretically by using the "stress–strain" method [38] within *ab initio* method, can be used to estimate its some mechanical properties and also to examine dynamical stability of it. The calculated elastic constants of a material can give more and detailed information about its mechanical and dynamical behaviors such as stability, hardness or stiffness of it. C_{11}, C_{12} and C_{44} are three independent elastic constants of a cubic crystal [39]. The calculated second order elastic constants of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys within both GGSA and LSDA are presented in Table 4. The mechanically stability of a crystal depends on its elastic constants which is called Born's stability criteria [40]. This criteria tell about strain energy of this crystal against any homogeneous elastic deformation and this energy value must be positive [41]. For a cubic crystal, Born's mechanical stability criterias are given by

$$C_{11} - C_{12} > 0; C_{11} + 2C_{12} > 0; C_{11} > 0; C_{44} > 0 \quad (3)$$

The calculated elastic constants within both GGSA and LSDA show that Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure are stable mechanically due to satisfy these stability criteria.

Table 2. The optimized structural parameters of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA and LSDA.

Material	GGSA			LSDA		
	a (Å)	B (GPa)	B′	a (Å)	B (GPa)	B′
Fe_3Al	5.748	160.99	4.375	5.560	213.96	4.598
Fe_3Ga	5.772	163.40	4.656	5.575	223.96	4.822
Fe_3Si	5.603	205.31	5.122	5.461	268.95	4.886
Fe_3Ge	5.733	177.59	5.296	5.568	242.73	5.072

Table 3. The total magnetic moment (μ) and partial magnetic moments of the atoms of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3–type structure within GGSA and LSDA.

Material	GGSA		LSDA	
	μ_{tot} (μ_B)	μ_{atom} (μ_B)	μ_{tot} (μ_B)	μ_{atom} (μ_B)
Fe_3Al	6.073	$\mu_{Fe_{A,C}}$ = 1.883 μ_{Fe_B} = 2.369 μ_{Al} = -0.061	3.827	$\mu_{Fe_{A,C}}$ = 0.888 μ_{Fe_B} = 2.071 μ_{Al} = -0.020
Fe_3Ga	6.075	$\mu_{Fe_{A,C}}$ = 1.914 μ_{Fe_B} = 2.398 μ_{Ga} = -0.151	5.005	$\mu_{Fe_{A,C}}$ = 1.471 μ_{Fe_B} = 2.143 μ_{Ga} = -0.079
Fe_3Si	5.110	$\mu_{Fe_{A,C}}$ = 1.320 μ_{Fe_B} = 2.517 μ_{Si} = -0.047	3.838	$\mu_{Fe_{A,C}}$ = 0.788 μ_{Fe_B} = 2.271 μ_{Si} = -0.009
Fe_3Ge	5.450	$\mu_{Fe_{A,C}}$ = 1.500 μ_{Fe_B} = 2.528 μ_{Ge} = -0.078	4.670	$\mu_{Fe_{A,C}}$ = 1.160 μ_{Fe_B} = 2.390 μ_{Ge} = -0.041

Additionally, some mechanical properties of a crystal such as bulk (B) and shear moduli (G), Young's modulus (E) and Poisson's ratio (ν), can be estimated by using its elastic constants. Voigt [42] - Reuss [43] - Hill [44] relations can be used to estimate the bulk (B) and shear moduli (G) of a crystal. Voigt approximation can be used to calculate the upper limits (B_V, G_V) and Reuss approximation can be used to estimate the lower limits (B_R, G_R) of B and G values of a crystal as in Eq.4-6, respectively.

$$B_V = B_R = B = (C_{11} + 2C_{12})/3 \quad (4)$$

$$G_V = (C_{11} - C_{12} + 3C_{44})/5 \quad (5)$$

$$G_R = 5(C_{11} - C_{12})C_{44}/(4C_{44} + 3C_{11} - 3C_{12}) \quad (6)$$

Hill approximation can be used to calculate the average values of bulk and shear moduli of a crystal which are given by $B = (1/2)(B_V + B_R)$ and $G = (1/2)(G_V + G_R)$, respectively. As seen in Eq.4, upper (B_V), lower limits (B_R) and average value (B) of a cubic crystal are equal to each other.

Moreover, the estimated bulk and shear moduli can be used to calculate Young's modulus (E) [41] and Poisson's ratio (ν) [41] of a cubic crystal as given by Eq.7 and Eq.8, respectively.

$$E = (9BG)/(3B + G) \quad (7)$$

$$\nu = (3B - 2G)/[2(3B + G)] \quad (8)$$

The calculated bulk modulus (B_V, B_R and B), shear modulus (G_V, G_R and G) and Young's modulus (E), B/G and k = G/B (Pugh's ratio) ratios [45] and the calculated Poisson's ratios (ν) of Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure within GGSA and LSDA are shown in Table 5 and 6, respectively.

The stiffness of a crystal can be determined with its Young's modulus (E) which is given as the ratio of stress and strain. The calculated shear and Young's moduli of our materials suggest that Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure are rather hard materials. Moreover, the calculated B/G and Pugh's ratios (k=G/B) indicate that these alloys are ductile materials.

It is known that if B/G of a material is ranging from 1.7 to 5.6 and Poisson's ratio is ranging from 0.25 to 0.42, this material show metallic behavior [46]. Therefore, Poisson's ratios and B/G values of Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure show that the bonding character of our materials are close to metallic.

To determine anisotropic or isotropic behavior of a crystal, shear anisotropy factors [47] can be used. The shear anisotropy factors (A and A_) in {100} and {110} planes of a cubic crystal can be calculated as in Eq.9 and Eq.10, respectively [47]:

$$A = 2C_{44}/(C_{11} - C_{12}) \quad (9)$$

$$A_- = C_{44}(C_L + 2C_{12} + C_{11})/(C_L C_{11} - C_{12}^2) \quad (10)$$

whereas $C_L = C_{44} + (C_{11} + C_{12})/2$.

These calculated values within GGSA and LSDA for Fe_3M (M=Al, Ga, Si and Ge) alloys are presented in Table 7 and 8, respectively. The shear anisotropy factors A and A_ of our alloys show that for (100) plane, are greater than that for (110) plane as seen in Table 7 and Table 8. All of our alloys in this study show largely mechanical anisotropy.

Table 4. The calculated second order elastic constants of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA and LSDA.

Material	GGSA			LSDA		
	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
Fe_3Al	208.46	158.80	140.75	305.42	205.67	171.50
Fe_3Ga	187.63	153.97	122.10	271.71	198.18	170.37
Fe_3Si	290.21	185.52	145.11	358.84	230.34	175.56
Fe_3Ge	187.27	152.37	129.57	296.68	194.57	146.62

Table 5. The estimated bulk moduli, upper and lower limits, average values of shear moduli, Young's moduli and Poisson's ratios of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure within GGSA.

Material	B (GPa)	G_V (GPa)	G_R (GPa)	G (GPa)	E (GPa)	B/G	k (G/B)	ν
Fe_3Al	175.35	94.38	49.09	71.73	189.38	2.44	0.409	0.320
Fe_3Ga	165.19	79.99	34.86	57.43	154.40	2.88	0.348	0.344
Fe_3Si	220.42	108.01	84.92	96.46	252.54	2.29	0.438	0.309
Fe_3Ge	164.00	84.72	36.30	60.51	161.65	2.71	0.369	0.336

Table 6. The estimated bulk moduli, upper and lower limits, average values of shear moduli, Young's moduli and Poisson's ratios of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure within LSDA.

Material	B (GPa)	G_V (GPa)	G_R (GPa)	G (GPa)	E (GPa)	B/G	k (G/B)	v
Fe_3Al	238.92	122.85	86.81	104.83	274.37	2.28	0.439	0.309
Fe_3Ga	222.69	116.93	69.44	93.18	245.33	2.39	0.418	0.316
Fe_3Si	273.17	131.03	103.70	117.37	307.99	2.33	0.430	0.312
Fe_3Ge	228.61	108.39	83.84	96.12	252.90	2.38	0.420	0.316

Table 7. The calculated anisotropy shear factors (A and A_) and longitudinal (v_l), transverse (v_t), and average (v_m) wave velocities in crystal and also Debye temperatures (Θ_D) of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure within GGSA.

Material	A	A_	v_l (m/s)	v_t (m/s)	v_m (m/s)	Θ_D (K)
Fe_3Al	5.668	2.823	6298.2	3240.4	3628.8	474.4
Fe_3Ga	7.255	3.081	5407.4	2635.5	2960.8	386.0
Fe_3Si	2.772	1.975	6878.2	3615.9	4043.6	541.3
Fe_3Ge	7.425	3.121	5357.2	2664.1	2989.6	392.2

Table 8. The calculated anisotropy shear factors (A and A_) and longitudinal (v_l), transverse (v_t), and average (v_m) wave velocities in crystal and also Debye temperatures (Θ_D) of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3 structure within LSDA.

Material	A	A_	v_l (m/s)	v_t (m/s)	v_m (m/s)	Θ_D (K)
Fe_3Al	3.439	2.226	7043.9	3706.1	4144.2	562.1
Fe_3Ga	4.634	2.581	6125.6	3174.6	3553.5	480.9
Fe_3Si	2.733	1.958	7336.2	3834.3	4289.4	589.5
Fe_3Ge	2.872	2.013	6222.1	3229.6	3614.6	486.7

It can be used Navier's equation [48] to calculate longitudinal and transverse wave velocities of a crystal. These values of Fe_3M (M=Al, Ga, Si and Ge) alloys are calculated by using Eq.11 and Eq.12 and also the average wave velocities [49] of these alloys were calculated by using Eq.13.

$$v_l = \left[\left(B + (4G/3)\right)/\rho\right]^{1/2} \quad (11)$$

$$v_t = [G/\rho]^{1/2} \quad (12)$$

$$v_m = \left\{(1/3)\left[\left(2/(v_t^3)\right) + \left(1/(v_l^3)\right)\right]\right\}^{-1/3} \quad (13)$$

where ρ is the density of the material. The sound velocity of Fe_3Si alloy is highest while Fe_3Ga alloy has lowest value as seen in Table 7 and Table 8.

Many physical properties such as specific heat and melting temperature has relation with the Debye temperature (Θ_D) of a crystal. Therefore it is an important fundamental parameter [50] and also in this study, we were calculated the Debye temperatures (Θ_D) of our alloys by using Eq.14 [51].

$$\theta_D = (h/k)[(3n/4\pi)(N_A\rho/M)]^{1/3}v_m \quad (14)$$

where h is the Planck's constant, k the Boltzmann's constant, N_A is the Avogadro's number, M is the molecular weight and n is the number of atoms in the molecule. The calculated Debye temperatures (Θ_D) of Fe_3M (M=Al, Ga, Si and Ge) alloys are presented in Table 7 and Table 8. This value of Fe_3Si alloy is higher than the others while Fe_3Ga has lowest Debye temperature as seen in Table 7 and Table 8.

3.4. Electronic band structures

The electronic behavior of a material is determined the calculated electronic band structure and the density of states (DOS) of it. The plotted electronic band structures and total density of states (DOS) of Fe_3M (M=Al, Ga, Si and Ge) alloys in both majority (up) and minority (down) spin channels within LSDA and GGSA are presented along the high symmetry lines in the first Brillouin zone, respectively, in Fig. 3. It can be clearly seen that, our materials show metallic behavior due to there is no band gap neither for up nor for down spin channels in electronic band structures within both LSDA and GGSA. Additionally, our materials have ferromagnetic nature and this situation is well in agreement with total magnetic moments of our alloys as seen in Table

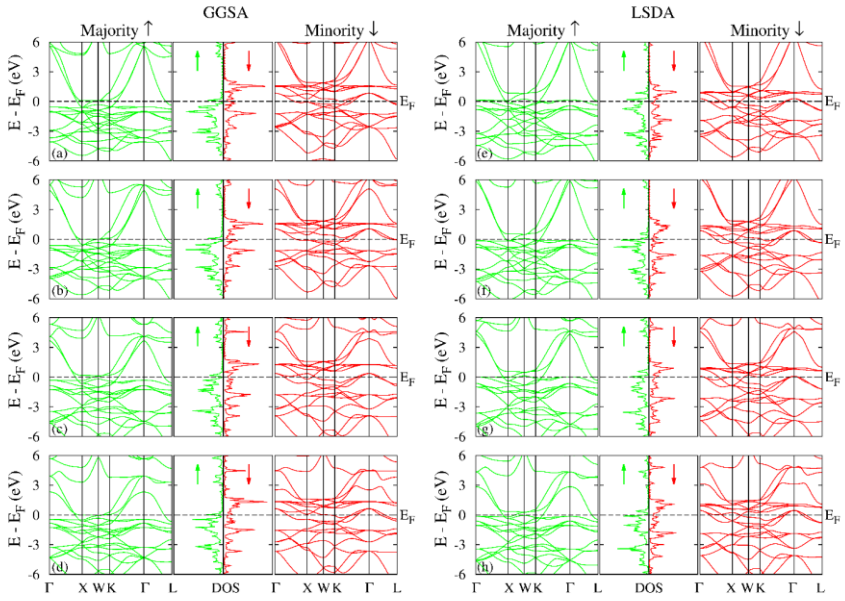

Fig. 3. The calculated energy band structures and the total density of electronic states (DOS) within GGSA for (a) Fe_3Al, (b) Fe_3Ga, (c) Fe_3Si, (d) Fe_3Ge and within LSDA for (e) Fe_3Al, (f) Fe_3Ga, (g) Fe_3Si, (h) Fe_3Ge alloys. The zero of band energy is shifted to Fermi level (E_F).

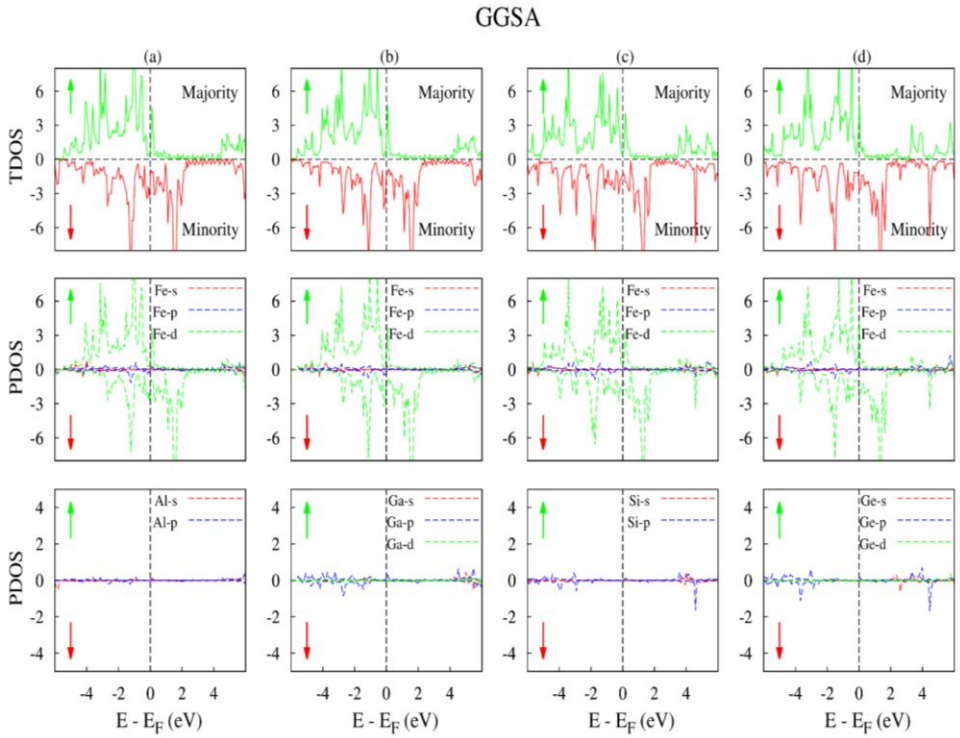

Fig. 4. The total and orbital projected partial density of electronic states of atoms within GGSA for (a) Fe_3Al, (b) Fe_3Ga, (c) Fe_3Si and (d) Fe_3Ge alloy.

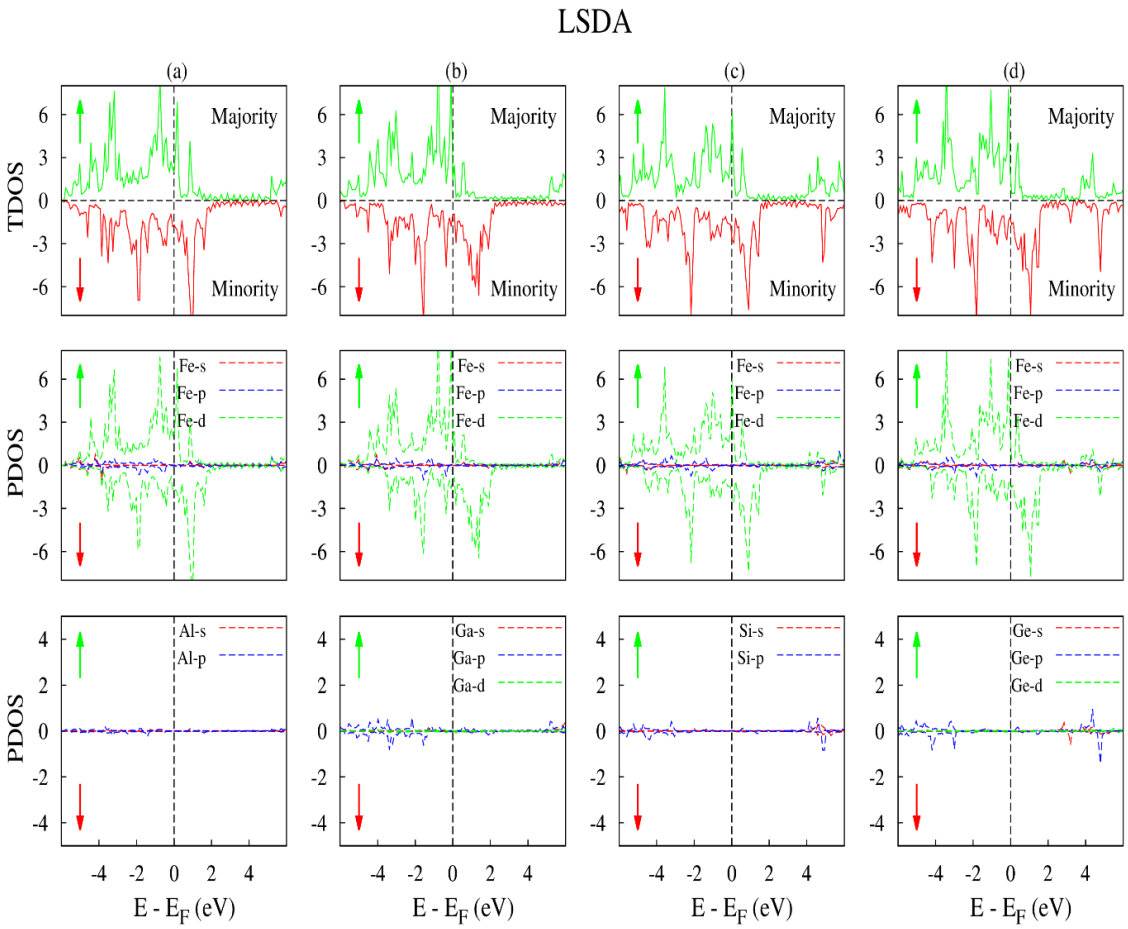

Fig. 5. The total and orbital projected partial density of electronic states of atoms within LSDA for (a) Fe_3Al, (b) Fe_3Ga, (c) Fe_3Si and (d) Fe_3Ge alloy.

The calculated orbital projected partial density of electronic states of atoms within GGSA and LSDA in Fe_3M (M=Al, Ga, Si and Ge) alloys are given in Figs. 4-5, respectively. For all of our materials, 3d states of Fe atoms cross the Fermi level (E_F), yielding a metallic behavior. In addition, we see that the p orbitals of M (M=Al, Ga, Si and Ge) atoms has no remarkable effect on bonding features of these systems. In this respect, the metallicity and the bonding properties of these systems can be attributed to d-orbitals of Fe atom in our compositions.

4. CONCLUSION

The structural, magnetic, mechanical properties and electronic band structure of full-Heusler Fe_3M (M=Al, Ga, Si and Ge) alloys in DO_3-type structure which conforms to $Fm\bar{3}m$ space group, have been examined in detail in ferromagnetic order and also showed differences between GGSA and LSDA. Especially, the calculated structural parameters for Fe_3M (M=Al, Ga, Si and Ge) alloys within GGSA are more accurate than within LSDA. The calculated spin-polarized electronic band structures within both GGSA and LSDA of our alloys show that all of our materials have metallic character and also are ferromagnets due to the differences between majority (up) and minority (down) spin channels. The calculated elastic constants and estimated mechanical properties of these alloys show that these alloys are stable mechanically and have largely anisotropic character.

ACKNOWLEDGMENTS

This work was supported by the Ahi Evran University Research Project Unit under Project No PYO-KMY.4001.15.001

REFERENCES

[1] Heusler F., **"*Über magnetische Manganlegierungen*"**, Verhandlungen der Deutschen Physikalischen Gesellschaft, German, 12: 219, (1903).

[2] Potter H. H., "***The X-ray Structure and Magnetic Properties of Single Crystals of Heusler Alloy***", Proceedings of Physical Society, 41: 135, (1928).

[3] Bradley A. J., Rogers J. W., "***The Crystal Structure of the Heusler Alloys***", Proceedings of The Royal Society A, 144 (852): 340, (1934).

[4] Franco V., Blazquez J. S., Ingale B., Conde A., ***"The Magnetocaloric Effect and Magnetic Refrigeration***

Near Room Temperature: Materials and Models", Annual Review of Materials Research, 42: 305, (2012).

[5] Entel P., Buchelnikov V. D., Khovailo V. V., Zayak A. T., Adeagbo W. A., Gruner M. E., Herper H. C., Wassermann E. F., ***"Modelling the phase diagram of magnetic shape memory Heusler alloys"***, Journal of Physics D: Applied Physics, 39: 865, (2006).

[6] Yu S. Y., Liu Z. H., Liu G. D., Chen J. L., Cao Z. X., Wu G. H., Zhang B., Zhang X. X., ***"Large magnetoresistance in single-crystalline Ni50Mn50-xInx alloys (x=14-16) upon martensitic transformation"***, Applied Physics Letters, 89: 162503, (2006).

[7] Muthu S. E., Rao N. V. R., Rao D. V. S., Raja M. M., Devarajan U., Arumugam S., ***"Effect of Ni/Mn concentration on exchange bias properties in bulk Ni50-xMn37+xSn13 Heusler alloys"***, Journal of Applied Physics, 110: 023904, (2011).

[8] Krenke T., Duman E., Acet M., Wassermann E. F., Moya X., Manosa L., Planes A., Suard E., Ouladdiaf B., ***"Magnetic superelasticity and inverse magnetocaloric effect in Ni-Mn-In"***, Physical Review B, 75: 104414, (2007).

[9] Zhang B., Zhang X. X., Yu S. Y., Chen J. L., Cao Z. X., Wu G. H., ***"Giant magnetothermal conductivity in the Ni–Mn–In ferromagnetic shape memory alloys"***, Applied Physics Letters, 91: 012510, (2007).

[10] Kübler J., Williams A. R., Sommers C. B., **"*Formation and coupling of magnetic moments in Heusler alloys*"**, Physical Review B, 28: 1745, (1983).

[11] Felser C., Fecher G. H., Balke B., ***"Spintronics: a challenge for materials science and solid-state chemistry"***, Angewandte Chemie (International ed. İn English), 46: 668, (2007).

[12] Jung D., Koo H. J., Whangbo M. H., ***"Study of the 18-electron band gap and ferromagnetism in semi-Heusler compounds by non-spin-polarized electronic band structure calculations"***, Journal of Molecular Structure (Theochem), 527: 113, (2000).

[13] Wernick J. H., Hull G. W., Geballe T. H., Bernardini J. E., Waszczak J. V., ***"Superconductivity in ternary Heusler intermetallic compounds"***, Materials Letters, 2: 90, (1983).

[14] Gasi T., Ksenofontov V., Kiss J., Chadov S., Nayak A. K., Nicklas M., Winterlik J., Schwall M., Klaer P., Adler P., Felser C. ***"Iron-based Heusler compounds Fe2YZ: Comparison with theoretical predictions of the crystal structure and magnetic properties"***, Physical Review B, 87: 064411, (2013).

[15] Felser C., Hirohata A., ***"Heusler Alloys: Properties, Growth, Applications"***, Springer Series in Materials Science, Switzerland, (2016).

[16] Raja M. M., Kamat S. V., ***"Structure, Magnetic, and Electrical Properties of Heusler-Type Fe3-xCoxSi Ferromagnetic Alloys"***, Metallurgical and Materials Transactions A, 46A: 4688, (2015).

[17] Kogachi M., Fujiwara T., Kikuchi S., ***"Atomic disorder and magnetic property in Co-based Heusler alloys Co2MnZ (Z=Si, Ge, Sn)"***, Journal of Alloys and Compounds, 475: 723, (2009).

[18] Miura Y., Nagao K., Shirai M., ***"Atomic disorder effects on half-metallicity of the full-Heusler alloys Co2(Cr1-xFex)Al: A first-principles study"***, Physical Review B, 69: 14413, (2004).

[19] Kandpal H. C., Ksenofontov V., Wojcik M., Seshadri R., Felser C., ***"Electronic structure, magnetism and disorder in the Heusler compound Co2TiSn"***, Journal of Physics D: Applied Physics, 40: 1587, (2007).

[20] Picozzi S., Continenza A., Freeman A. J., ***"Role of structural defects on the half-metallic character of Co2MnGe and Co2MnSi Heusler alloys"***, Physical Review B, 69: 094423, (2004).

[21] Kresse G., Hafner, J., ***"Ab initio molecular dynamics for liquid metals"***, Physical Review B, 47: 558, (1994).

[22] Kresse G., Furthmüller J., ***"Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set"***, Computational Material Science, 6: 15, (1996).

[23] Blöchl P. E., ***"Projector augmented-wave method"***, Physical Review B, 50: 17953, (1994).

[24] Kresse G., Joubert J., ***"From ultrasoft pseudopotentials to the projector augmented wave method"***, Physical Review B, 59: 1758, (1999).

[25] Perdew J. P., Zunger A., ***"Self-interaction correction to density-functional approximations for many-electron systems"***, Physical Review B, 23: 5048, (1981).

[26] Perdew J. P., Burke K., Ernzerhof M., ***"Generalized Gradient Approximation Made Simple"***, Physical Review Letters, 77: 3865, (1996).

[27] Kohn W., Sham L. J., ***"Self-Consistent Equations Including Exchange and Correlation Effects"***, Physical Review, 140: A1133, (1965).

[28] Hohenberg P., Kohn W., ***"Inhomogeneous Electron Gas"***, Physical Review, 136: B864, (1964).

[29] Monkhorst H. J., Pack J. D., ***"Special points for Brillouin-zone integrations"***, Physical Review B, 13: 5188, (1976).

[30] Vinet P., Rose J. H., Ferrante J., Smith J. R., ***"Universal Features of the Equation of State of Solids"***, Journal of Physics: Condensed Matter, 1: 1941, (1989).

[31] Feng J., Xiao B., Chen J. C., Zhou C. T., ***"Theoretical study on the stability and electronic property of Ag2SnO3"***, Solid State Sciences, 11: 259, (2009).

[32] Matar S. F., Weihrich R., Kurowski D., Pfitzner A., ***"DFT calculations on the electronic structure of CuTe2 and Cu7Te4"***, Solid State Sciences, 6: 15, (2004)

[33] Rausch J. B., Kayser F. X., ***"Elastic constants and electrical resistivity of Fe3Si"***, Journal of Applied Physics, 48: 487, (1977).

[34] Moroni E. G., Wolf W., Hafner J., Podlocky R., ***"Cohesive, structural, and electronic properties of Fe-Si compounds"***, Physical Review B, 59: 12860, (1999).

[35] Hsu L. S., Wang Y. K., Guo G. Y., Lue C. S., ***"Experimental and theoretical study of the electronic structure of Fe3Al, Fe2VAl, and Fe2VGa"***, Physical Review B, 66: 205203, (2002).

[36] Christensen N. E., Kudrnovsky J., Rodriguez C. O., ***"Metamagnetic behavior in Fe3Si and Fe3Al"***, International Journal of Material Science, 1: 1-15, (2007).

[37] Paduani C., Bormio-Nunes C., ***"Density functional theory study of Fe3Ga"***, Journal of Applied Physics, 109: 033705, (2011).

[38] Page Y. L., Saxe P., ***"Symmetry-general least-squares extraction of elastic coefficients from ab initio total energy calculations"***, Physical Review B, 63: 174103.1, (2001).

[39] Grimvall G., ***"Thermophysical Properties of Materials"***, Elsevier, New York, (1999).

[40] Mouhat F., Coudert F. X., ***"Necessary and Sufficient Elastic Stability Conditions in Various Crystal Systems"***, Physical Review B, 90: 224104, (2014).

[41] Wu D. H., Wang H. C., Wei L. T., Pan R. K., Tang B. Y., ***"First-principles study of structural stability and elastic properties of MgPd3 and its hydride"***, Journal of Magnesium and Alloys, 2: 165, (2014).

[42] Voigt W., ***"Lehrbuch der Kristallphysik"***, Springer, Berlin, (1928).

[43] Reuss A., ***"Berechnung der Fliessgrenze von Mischkristallen auf Grund der Plastizitätsbedingung für Einkristalle"***, Journal of Applied Mathematics and Mechanics, 9: 49, (1929).

[44] Hill R., ***"The Elastic Behaviour of a Crystalline Aggregate"***, Proceedings of the Physical Society Section A, 65: 349, (1952).

[45] Pugh S. F., ***"XCII. Relations between the elastic moduli and the plastic properties of polycrystalline pure metals"***, Philosophical Magazine Series 7, 45: 823, (1954).

[46] Greaves G. N., Greer A. L., Lakes R. S., Rouxel T., ***"Poisson's ratio and modern materials"***, Nature Materials, 10: 823, (2011).

[47] Lau K., McCurdy A. K., ***"Elastic anisotropy factors for orthorhombic, tetragonal, and hexagonal crystals"***, Physical Review B, 58: 14, (1998).

[48] Schreiber E., Anderson O. L., Soga N., ***"Elastic Constants and Their Measurements"***, McGraw-Hill, New York, (1973).

[49] Anderson O. L., ***"A simplified method for calculating the debye temperature from elastic constants"***, Journal of Physics and Chemistry of Solids, 24: 909, (1963).

[50] Johnston I., Keeler G., Rollins R., Spicklemire S., ***"Solid State Physics Simulations (Consortium for Upper-Level Physics Software)"***, Wiley, New York, (1996).

[51] Deligoz E., Colakoglu K, Ciftci Y. O., ***"Ab Initio Study on Hypothetical Silver Nitride"***, Chinese Physics Letters, 25: 2154, (2008)