
**STRUCTURE OF MATTER
AND QUANTUM CHEMISTRY**

First-Principle Investigations of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ Alloys. A Study on Structural, Magnetic, Electronic, and Elastic Properties

O. Örnek^{a,*}, A. İyigör^b, A. S. Meriç^a, M. Çanlı^c, M. Özduran^d, and N. Arıkan^{e,**}

^a Department of Materials and Metallurgical Engineering, Kırşehir Ahi Evran University, Kırşehir, 40200 Turkey

^b Department of Machinery and Metal Technology, Kırşehir Ahi Evran University, Kırşehir, 40100 Turkey

^c Department of Chemistry and Chemical Processing Technologies, Kırşehir Ahi Evran University, Kırşehir, 40500 Turkey

^d Department of Physics, Faculty of Arts and Sciences, Kırşehir Ahi Evran University, Kırşehir, 40200 Turkey

^e Department of Medical Services and Techniques, Osmaniye Korkut Ata Universit, Osmaniye, 80010 Turkey

* e-mail: osmanornek@ahievran.edu.tr

** e-mail: nihatarikan@osmaniye.edu.tr

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Abstract—The structural, magnetic, electronic and elastic properties of ternary and quaternary $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ alloys with inverse-Heusler (XA) structure were investigated at $x = 0, 0.25, 0.50, 0.75,$ and 1 . The crystal structures of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ compounds are cubic (space group: $F\bar{4}3m$) with Hg_2CuTi prototype for $x = 0$ and 1 . At $x = 0.5$ the structure is also cubic (space group: $F\bar{4}3m$) with LiMgPdSn prototype, while it is tetragonal (space group: $P\bar{4}m2$) at $x = 0.25$ and 0.75 . Calculated optimized lattice parameters (a and c), bulk modulus (B), and elastic constants (C_{ij}) are consistent with the available data in the literature. Total and partial magnetic moments of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ alloys were obtained. An increase in the total magnetic moment values were observed upon addition of V to the Ti_2FeGa alloy. From spin polarized band calculations, Ti_2FeGa , $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$, TiVFeGa , and V_2FeGa have a minority-spin energy gap of $0.65, 0.38, 0.83,$ and 0.64 eV, respectively, and they are guessed as half-metallic ferromagnets. According to the results of second-order elastic constants, these compounds met the Born mechanical stability criteria. In addition, according to Pugh criteria, it was found that they have a ductile structure and show anisotropic behavior.

Keyword: ab initio calculations, band calculations, mechanical properties, Heusler phase

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INTRODUCTION

Heusler alloys are widely studied since their discovery in 1903 [1]. Spin electrons on the alloys allow them to be used for especially in conducting magnetism, ferromagnetic shape memory [1, 2]. In the basis of Heusler alloys, non-ferromagnetic materials turn out to be ferromagnetic alloys with high Curie temperature which have capacity of being used in spintronics industry. There are three types of phases according to their positioning called full-Heusler alloys (X_2YZ) with $L2_1$ (no. 225) crystal structure, inverse-Heusler alloys (X_2YZ) with XA (no. 216) crystal structure and half-Heusler alloys (XYZ) with $C1_b$ (no. 216) crystal structure. The full Heusler compounds are ternary intermetallics with a $2 : 1 : 1$ stoichiometry (X_2YZ) in which X and Y are transition metals and Z is the main group element.

Bacon and Plant [3] created possible scenarios for both X_2YZ and XYZ chemical ordering. Heusler alloys consist of four face-centered cubic sublattices, which

can be characterized by the Wyckoff coordinates A (0, 0, 0), B (0.25, 0.25, 0.25), C (0.5, 0.5, 0.5), and D (0.75, 0.75, 0.75). Since most of the Heusler alloys are half metallic, they are categorized as crystallizing in $L2_1$ structure. Their space group can be either $Fm\bar{3}m$ (full Heusler) or $F\bar{4}3m$ (inverse Heusler) [2, 4, 5]. Inverse Heusler materials can be obtained in structure XA (X_2YZ) by replacing one of the X atoms of one of the full Heusler materials in the structure of $L2_1$ with the Y or Z atom and have $F\bar{4}3m$ space group; so, it is necessary to investigate the effect of site occupation on the half-metallicity of Heusler alloys. Wei et al. [6] found Ti_2 -based compounds as insensitive to the lattice distortion with fully spin polarization. Liping et al. [7] focused on searching structural, electronic, and magnetic properties of Ti_2FeGa . The bonds between $\text{Ti(A)}-\text{Ti(B)}$ coupling and Fe atoms come from electron hybridization of the d states which lies on the band gaps. According to Drief et al. [8], the gap energy

equal to 0.60 eV for Ti_2FeGa , in the spin-down state and divulge metallic intersections at the Fermi level for the spin-up state. Zhang et al. [1] found Ti_2FeGa is most likely to form Cu_2MnAl -type structure. Besides, Goraus and Czerniewski [9] characterize Ti_2FeGa as a material with ferromagnetic ordering within the 30–50 K range, with the latter showing some spin glass type behavior, and metallic type density of states.

Although some of the structural features of Ti_2FeGa alloy has been studied in terms of their theoretical aspects, the vanadium doped properties of this alloy have not been investigated at sufficient levels. Unique band structures can be observed in most of the vanadium based inverse-Heusler compounds. In these compounds, there is a higher opportunity to get half-metallic ferromagnetism (HMFs). None of the previous studies has investigated quadratic elastic constants and their respective elastic properties. One of the main problems in estimating the properties of materials is finding an accurate ab-initio method for simulation modeling of materials. Simulation allows discovering some properties that have not yet been experimentally investigated or are difficult to measure experimentally.

In this study, the Ti_2FeGa inverse-Heusler alloy, which has a limited number of studies in the literature, was added with various ratios of V atoms to get $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys. Structural, electronic, magnetic and mechanical properties of these alloys were determined in Density Functional Theory (DFT) by using GGY-PBE pseudopotentials. There was no prior study in literature about the alloys formed by selecting $x = 0.25, 0.5, 0.75$ ratios. Therefore, this study will provide an insight into structural, magnetic, electronic and mechanical properties of these alloys.

CALCULATION METHODOLOGY

The MedeA-VASP software package [10, 11] was used for DFT calculations with the projected augmented-wave (PAW) potentials. The generalized gradient approximation (GGA) of Perdew–Burke–Ernzerhof (PBE) [12] was performed for the exchange–correlation energy function. The stable structures that can be formed when V atom is added instead of Ti atom by using MedeA: Substitutional Search module are determined as $P\bar{4}m2$ tetragonal structure for $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeG}$, and cubic structure ($F\bar{4}3m$) for Ti_2FeGa , TiVFeGa , and V_2FeGa . A plane-wave basis set with a 500 eV energy cut-off was employed for the spin-polarized calculation of structural, electronic, and elastic properties. The energy convergence criteria were arranged to value 10^{-10} eV using the Normal (blocked Davidson) algorithm and reciprocal space projection operators. The k -points created with gamma-points were performed on $8 \times 8 \times 8$ in the total energy calculation for the $F\bar{4}3m$ cubic structures

and on $12 \times 12 \times 12$ in the state density calculation, and on $8 \times 8 \times 6$ in the total energy calculation for the $P\bar{4}m2$ tetragonal structure and on $10 \times 10 \times 7$ in the state density calculation. The Fermi distribution function with a smearing parameter of 0.2 eV was employed to integrate the bands at Fermi level [13]. Elastic constant was calculated via stress-strain technique [14].

RESULTS AND DISCUSSION

Ti_2FeGa ($x = 1$) and V_2FeGa ($x = 0$) alloys crystallize in XA or Hg_2CuTi prototype structure (space group: $F\bar{4}3m$). The TiVFeGa ($x = 0.5$) alloy crystallizes LiMgPdSn in the cubic structure ($F\bar{4}3m$ space group) as a prototype. Alloys of $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeG}$ ($x = 0.25$) and $(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeG}$ ($x = 0.75$) composition crystallize in the tetragonal phase. All three phases were presented in Fig. 1. In the first step, $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ alloy's lattice parameters (a and c), the bulk module (B) and formation energy (ΔH_f) were calculated (Table 1) and compared to available data.

The calculated lattice constants and formation energies of the cubic alloys in the $F\bar{4}3m$ space group and tetragonal alloys in the $P\bar{4}m2$ space group are shown in Table 1. Computed lattice constants of Ti_2FeGa and V_2FeGa inverse Heusler alloys were compared with other theoretical studies in the literature. According to this, the lattice constant value obtained for the Ti_2FeGa alloy was determined with a difference of 0.02% from a GAST-PW91 using the CASTEP package program [1] and from the study GGY-PBE using the VASP program package, and with a difference of 1.3% from GGY-WC using the WIEN2k program package calculated by Drief et al. [8]. In addition, the lattice constant of the Ti_2FeGa alloy was experimentally obtained with a difference of 1.2% in the experimental and theoretical study of Goraus and Czerniewski. The lattice constant value of the V_2FeGe alloy differs by 0.18% from the value obtained by Ma et al. [15] using the VASP codes according to the GGY-PBE method, and with a difference of 0.17% from the value obtained by Zhang et al. [16] with the CASTEP program package according to the GGY method. There has been no comparison made for the TiVFeGa ($\text{Ti}_{0.75}\text{V}_{0.25}$) $_2\text{FeGa}$ and $(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$ alloys, since no studies have been found in the literature.

In Table 1, considering the lattice constants of the alloys, for the cubic structure at $x = 0, 0.5, 1$, with increase in vanadium content, the lattice constant values decreases. For the structures with tetragonal symmetry ($x = 0.25$ and 0.75), it is clearly seen that both the a and c lattice constant and the c/a ratio decrease upon addition of vanadium. This is caused by the fact that the atomic diameter of vanadium is lower than that of titanium.

The formation energy is a significant parameter which gives deep insight about whether studied compound is structurally stable and experimentally synthesizable or not [17]. The formation energy of Ti_2FeGa can be obtained from the following equation:

$$\Delta H_f = E_{\text{Ti}_2\text{FeGa}} - [2E_{\text{Ti}} + E_{\text{Fe}} + E_{\text{Ga}}],$$

where $E_{\text{Ti}_2\text{FeGa}}$ is the equilibrium total energy, E_{Ti} , E_{Fe} , and E_{Ga} are the energies per atom. As the computed formation energy value is negative, these compounds are thermodynamically stable and may be synthesized experimentally.

Considering the spin additive, the calculations were made according to spin polarizations for $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys. Slater–Pauling behavior (SPB) containing information on total magnetic moments can be applied for Heusler alloys. Since the 9 valence bands of the alloys in the Heusler structure ($x = 0, 0.5, 1$) examined in this study are full, the total magnetic moment according to SPB can be found by the rule of $M_t = (Z_t - 18)\mu_B$ [16, 17]. Z_t is the sum of the valence electrons in each atom forming the alloy or the sum of the number of electrons in the spin orbits as ($Z_t = N\uparrow + N\downarrow$). When total magnetic moments are calculated according to SPB, it is $1 \mu_B$ for Ti_2FeGa inverse-Heusler alloy, $2 \mu_B$ for TiVFeGa four-Heusler alloy, and as $3 \mu_B$ for V_2FeGa inverse-Heusler alloy. It is clearly seen in Table 2 that the total magnetic moments belonging to these Heusler alloys ($x = 0, 0.5, 1$) obtained because of calculations are in agreement with the values in the literature and the values obtained from the SPB. However, it may not always be true to say that $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$ and $(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$ alloys in the tetragonal structure are compatible with SPD. Therefore, no comparison was made for these alloys in tetragonal structure by applying the SPD rule. Nevertheless, there is an increase observed in the total magnetic moment values with increasing contribution of the V atom to the Ti_2FeGa alloy. Since the total magnetic moments of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys have non-zero values, spin orientations, electronic band curves, and state intensities are antisymmetrical. The greatest contribution to the total magnetic moments of these alloys comes from d orbitals of Ti, V, and Fe atoms which form the alloys when the partial state density curves are examined.

Many of the physical properties of solids are directly or indirectly related to the electronic band structure. In the electronic band structure of half-metal alloys, one spin-oriented electrons are conductive, while the other spin-oriented electrons act as insulators or semiconductors. Electronic band structures of the alloys of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) are given in Fig. 2. Examination of these electronic band curves showed that there is no forbidden energy range in the Fermi energy level and the bands

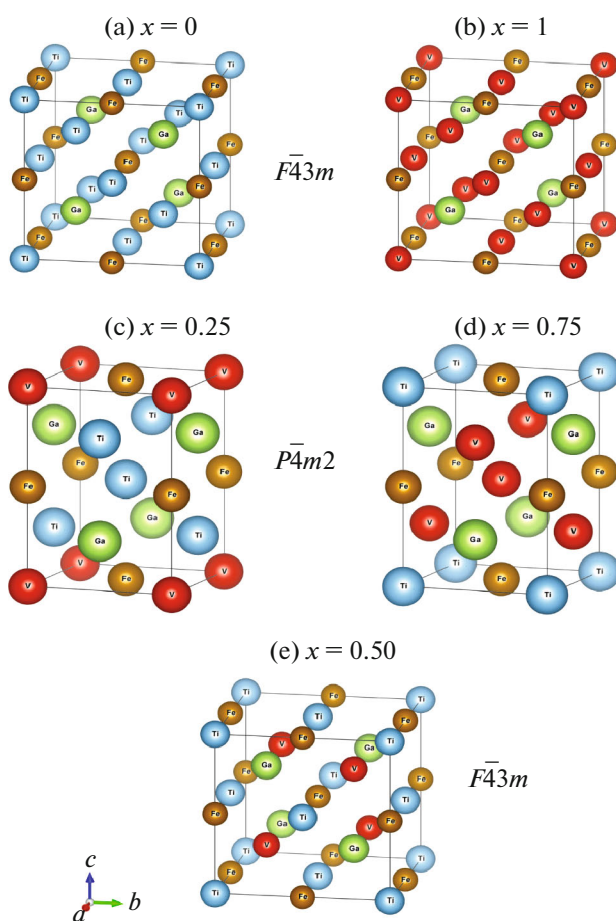


Fig. 1. Structures (a, b) for $x = 0$ and 1 the space group $F\bar{4}3m$ inverse-Heusler alloys, (c, d) tetragonal and belongs to the space group $P\bar{4}m2$, (e) the quadruple Heusler structure in the $F\bar{4}3m$ space group.

overlap the Fermi energy level in the spin up orientation of the inverse and quadruple Heusler alloys with $x = 0, 0.5, 1$. Therefore, it can be said that these alloys show metallic properties in spin up direction. In spin down orientation, Ti_2FeGa , $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$, TiVFeGa , and V_2FeGa alloys have a band gap around the Fermi level, and these alloys show a semiconductor feature in the spin down state. In this case, these four alloys exhibit half-metallic behavior. Also these alloys have an indirect band gap between valence and conductivity bands. The band gap values of these alloys are presented in Table 2. It was observed that the inverse-Heusler alloy Ti_2FeGa has the band gap values compatible to the data found in the available literature [18, 19]. However, there is no data in the literature to compare a band gap value for other alloys with. In addition, the $(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$ tetragonal alloy has a small band gap just below the Fermi energy level in the spin downward direction. This is because the tetragonal alloy exhibits only a half-metallic behavior.

Table 1. Calculated structural parameters (a , c in Å; V in Å³) and formation enthalpy (ΔH_f), eV/atom)

Materials	Ref.	a	c	c/a	V	ΔH_f
Ti ₂ FeGa	This study	6.101	—	—	227.119	−0.372
	Exam. [9]	6.177	—	—	—	
	GGY-PBE [13]	6.122	—	—	—	
	GGY-PBE [6]	6.120	—	—	—	
	GGY-PBE [7]	6.100	—	—	—	
	GGY-WC [8]	6.0226	—	—	—	
	PW [7]	6.177	—	—	—	
	GGY-PW91 [1]	6.100	—	—	—	
(Ti _{0.75} V _{0.25}) ₂ FeGa	This study	4.246	6.150	1.448	110.857	−0.360
TiVFeGa	This study	5.995	—	—	215.464	−0.277
(Ti _{0.25} V _{0.75}) ₂ FeGa	This study	4.210	5.951	1.413	105.478	−0.268
V ₂ FeGa	This study	5.921	—	—	207.656	−0.282
	GGY-PBE [13]	5.910	—	—	—	
	CASTEP-GGY [14]	5.911	—	—	—	

Table 2. (Ti_{1-x}V_x)₂FeGa ($x = 0, 0.25, 0.5, 0.75, 1$) alloys total and partial magnetic moments (M_i ; μ_B) and forbidden energy ranges in spin-down direction (E_g , eV)

Materials	Ref.	M_T	$M_{a-Ti(V)}$	$M_{b-V(Ti)}$	M_{Fe}	M_{Ga}	E_g
Ti ₂ FeGa	This study	1.0074	0.998	0.754	−0.941	0.000	0.65
	GGY-PBE [13]	1	1.005	0.757	−0.966	0.009	0.57
	GGY-PBE [6]	1	1.22	0.93	−1.09	−0.06	0.56
	GGY-PBE [2]	—	—	—	—	—	0.56
	GGY-PBE [7]	1.002	1.123	0.904	−1.196	0.008	0.59
	GGY-WC [8]	1.0016	0.7886	0.5026	—	0.00537	0.64
	GGY-PW91 [1]	0.98	1.00	0.76	−0.86	0.08	0.56
	(Ti _{0.75} V _{0.25}) ₂ FeGa	This study	1.5024	0.560	0.983	−0.440	−0.002
TiVFeGa	This study	1.8025	0.829	0.558	0.244	−0.008	0.83
(Ti _{0.25} V _{0.75}) ₂ FeGa	This study	1.9901	0.337	0.764	0.725	−0.005	0
V ₂ FeGa	This study	2.8365	1.698	−0.226	1.182	−0.010	0.64
	GGY-PBE [13]	2.8487	1.803	−0.231	1.200	−0.001	—
	CASTEP-GGY [14]	2.86	2.34	−0.50	1.18	−0.16	—

The total state intensity (TDOS) and partial state intensity (PDOS) was calculated to characterize the electronic band structures of the (Ti_{1-x}V_x)₂FeGa ($x = 0, 0.25, 0.5, 0.75, 1$) alloys in more detail. Figure 3 shows the TDOS and PDOS diagrams calculated for different (Ti_{1-x}V_x)₂FeGa ($x = 0, 0.25, 0.5, 0.75, 1$) alloys.

Considering the spin up bands of the five alloys, whose total and partial state densities are examined, the highest contribution to the Fermi level was the electrons from the d -states of the alloys. In the alloys of (Ti_{1-x}V_x)₂FeGa ($x = 0, 0.25, 0.5, 0.75, 1$), while $x = 0, 0.5, 1$ contributed the inverse and quaternary Heusler alloys had dominant Ti- d orbital electrons,

increase in the addition rate of the V atom showed similar pattern in the contribution of Fe- d orbital (states). When $x = 0.25$ or 0.75 , the contribution of the Fe- d orbital decreases in contrast to the cubic phase with the increase of the V atom in tetragonal alloys. In addition, these findings were compatible with the studies in the literature considering the electronic properties [1, 6–8, 15, 16].

Elastic constants (C_{ij}) give information about the strength of a material and its resistance to external forces. Elastic properties of solids are closely related to many physical properties such as melting point, heat capacity, thermal expansion coefficient, and Debye temperature. The materials with the cubic structure

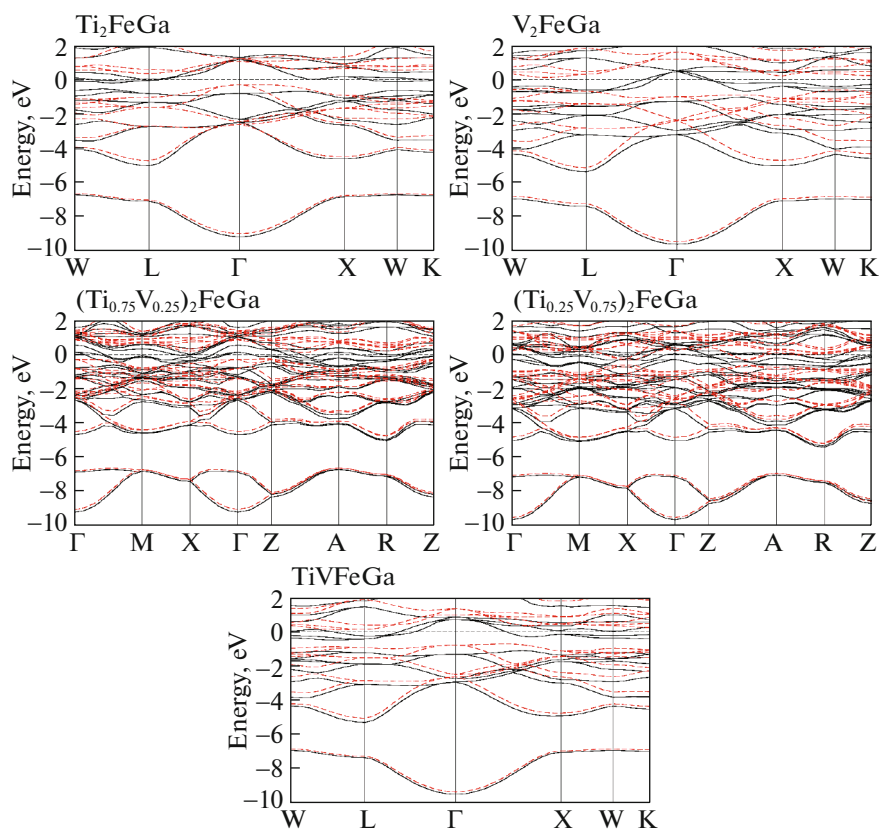


Fig. 2. Spin-polarized electronic band curves of the alloy $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ (the Fermi level is set to zero energy).

have three elastic constants, such as the second order C_{11} , C_{12} , and C_{44} , independent of each other. Tetragonal materials have six elastic constants, such as C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} , which are independent of each other. Calculated C_{ij} elastic constants for $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys are summarized in Table 3. Born mechanical stability criteria for elastic constants are expressed for cubic crystals as following equation:

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

and for crystals in tetragonal structure [20, 21]:

$$\begin{aligned} C_{11} > |C_{12}|, \quad 2C_{13}^2 < C_{33}(C_{11} + C_{12}), \\ C_{44} > 0, \quad C_{66} > 0. \end{aligned} \quad (2)$$

Considering values of C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} in Table 3, all of these alloys met the mechanical stability conditions. Therefore, both cubic inverse and quaternary Heusler alloys and tetragonal alloys can be considered mechanically stable in crystal symmetries. At the same time, when the elastic constants values of these alloys are examined, the C_{11} value increases with the increasing contribution of the V atom for all the alloys. In C_{12} value, it can be said that cubic alloys increase among themselves and tetragonal alloys among themselves in proportion with V contribution. In addition, the V_2FeGa alloy is the highest in C_{11} , C_{12} ,

and C_{44} values in the elastic constants among these alloys. Since there are no experimental or theoretical data about elastic constants for these alloys in the literature, no comparison could be done. Thus, elastic constants and related mechanical properties of these alloys are first time presented in this study.

The calculated elastic constants of the $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys were used for finding bulk module (B), shear modulus (G), Young modulus (E), Poisson ratio (σ), and anisotropy factor (A) and presented in Table 4. Bulk module values of these alloys were between C_{11} and C_{12} elastic constant values as expected. The bulk modulus value of the Ti_2FeGa inverse-Heusler alloy was compatible with a difference of 0.7% from Wei et al. [6] and with a slightly higher difference from other studies. Besides, the bulk modulus value increased in direct proportion to the V fraction in the Ti_2FeGa alloy. As an expression of compressibility, the shear module, G , the studied alloys were found to be more compressible since these alloys had a value below 100 GPa. It can also be said that the inverse-Heusler Ti_2FeGa alloy with the lowest shear modulus value is more compressible than the other alloys. In order to obtain information about the fragile or ductile nature of materials, Pugh's criterion was used. According to this criterion, if the B/G ratio is less than 1.75, the material is fragile, and if the

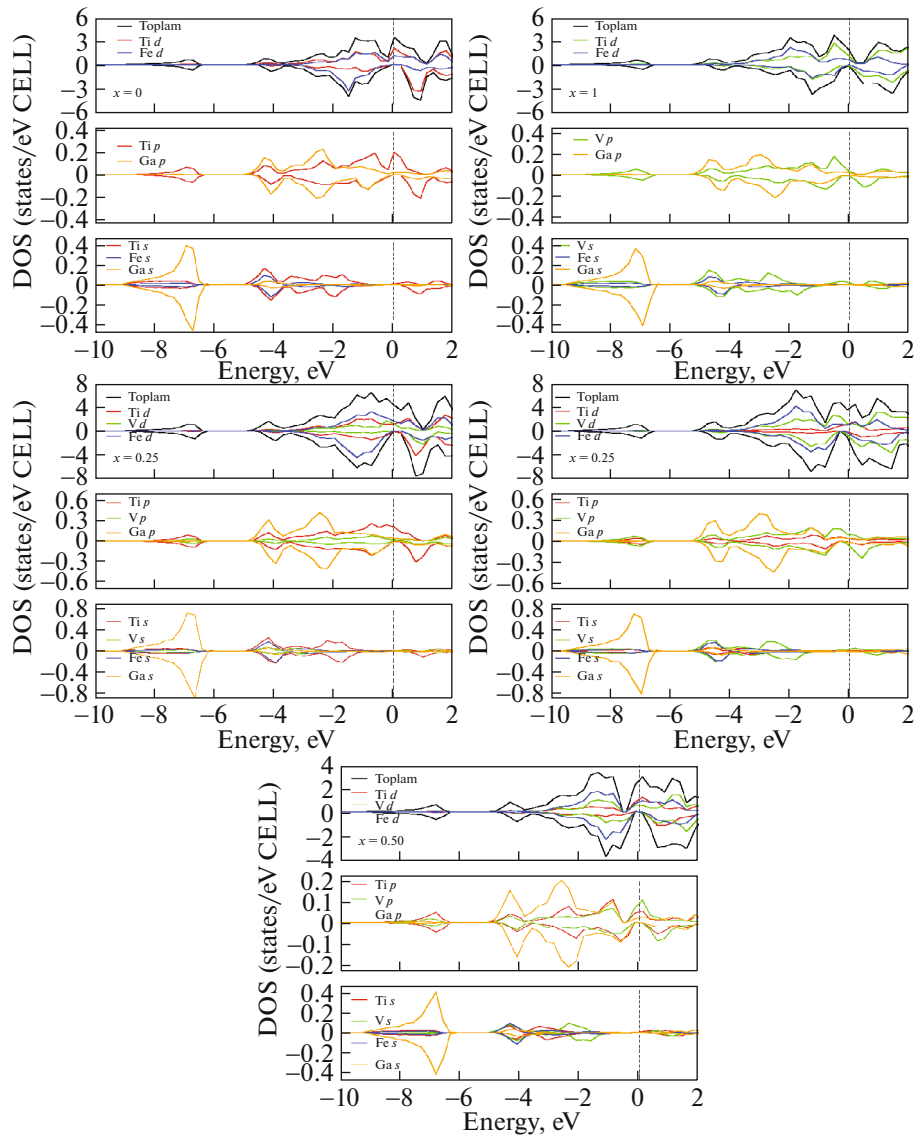


Fig. 3. Total and partial state intensities of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ alloys.

ratio is higher, it has a ductile nature. Accordingly, since the B/G ratio of these alloys is greater than 1.75, they are all ductile. For Heusler alloys with cubic crystal structure, the ductility decreases with increase in V fraction. For the alloys with $x = 0.25, 0.75$ having

tetragonal crystal structure, the ductility increases with increase in V content (Table 4).

Considering the Young's module, which is an expression of stiffness, in contrast to the B/G ratio, the hardness increases with increase in V content for the

Table 3. $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys in second order elastic constants (C_{ij} , GPa)

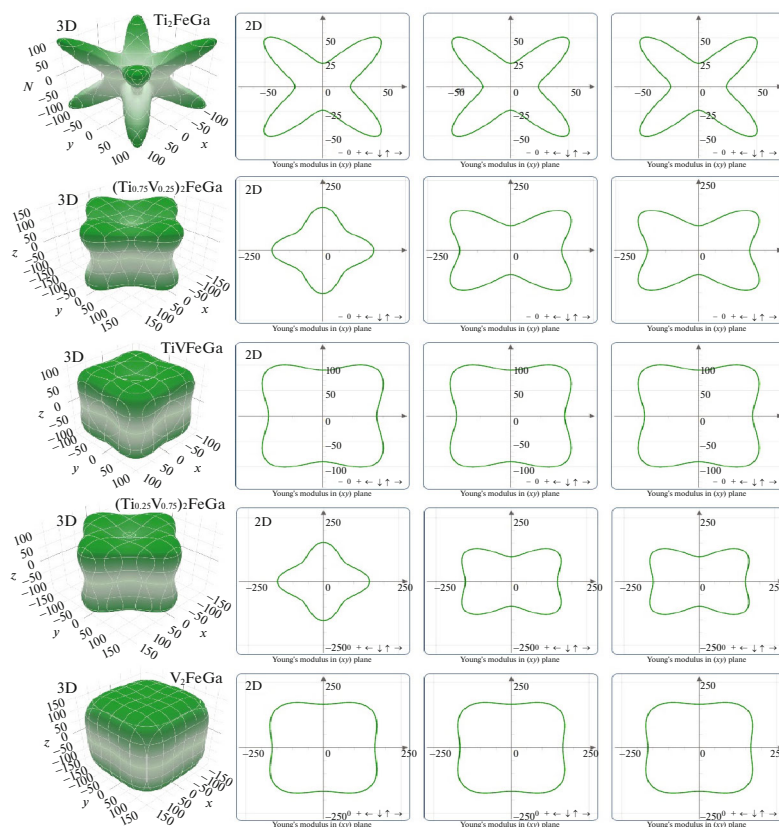
Materials	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
Ti_2FeGa	137.34	121.06	—	—	75.98	—
$(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$	236.53	80.77	122.68	181.79	92.77	37.41
TiVFeGa	202.57	138.74	—	—	55.89	—
$(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$	245.21	94.25	139.11	211.46	73.54	38.81
V_2FeGa	253.68	130.24	—	—	91.23	—

Table 4. Bulk modulus (B , GPa), shear modulus (G), B/G , Young modulus (E), Poisson ratio (σ), and anisotropy factor (A) of the studied alloys

Materials	Ref.	B , GPa	G , GPa	B/G	E , GPa	σ	A
Ti_2FeGa	This study	126.49	33.19	3.81	91.57	0.38	9.32
	GGY-PBE [6]	125.60					
	GGY-PBE [7]	172.63					
	GGY-WC [8]	152.74					
$(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$	This study	145.14	60.22	2.41	158.70	0.32	2.82
TiVFeGa	This study	160.01	44.64	3.58	122.53	0.37	1.75
$(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$	This study	160.69	55.78	2.88	149.99	0.34	2.14
V_2FeGa	This study	171.39	78.00	2.19	203.18	0.30	1.48

cubic structures, and the hardness decreases with increase in V fraction for the tetragonal structures. The calculated Poisson's ratio contains general information about atomic bonding. The value of the Poisson's ratio is close to 0.1 in covalent materials and close to 0.25 in ionic materials [22, 23]. The calculated Poisson's ratios of these alloys are between 0.30 and 0.38. Since this values are closer to 0.25, they appear to exhibit ionic character.

Another parameter obtained within the scope of mechanical properties is anisotropy factor. Anisotropy factor is equal to 1 for isotropic materials. Thus, the two- and three-dimensional dependences of the Young module were calculated for all materials using the ELATE program [24] and presented in Fig. 2. The plots for isotropic materials have spherical shape. The amount of deviation in Fig. 2 indicates the degree of anisotropy. As can be clearly seen from all planes in Fig. 4, all alloys are anisotropic.

**Fig. 4.** Three-dimensional (3D) and two-dimensional (2D) directional dependences of the Young's modulus of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ alloys.

CONCLUSIONS

The structural, magnetic, electronic, and elastic properties of $(\text{Ti}_{1-x}\text{V}_x)_2\text{FeGa}$ ($x = 0, 0.25, 0.5, 0.75, 1$) alloys were calculated using the generalized gradient approach with the Density Functional Theory. Considering lattice constants of the alloys among themselves, $x = 0, 0.5, 1$ in the cubic structure, the lattice constant values decrease with increase in V content. For structures at $x = 0.25$ and 0.75 with tetragonal symmetry, both a and c lattice constants and the c/a ratio decrease with increase in V content. This is caused by the fact that the atomic diameter of V is lower than that of Ti. The bulk modulus value of the Ti_2FeGa inverse-Heusler alloy is in good agreement with other theoretical studies. There was no available data to compare bulk modulus values calculated for other alloys. Total and partial spin magnetic moments of all the alloys were calculated and found that the calculated total and partial spin magnetic moments of all the cubic alloys were in good agreement with other theoretical calculations and Slater–Pauling rule. No comparison was made for the alloys with the tetragonal structure by applying the Slater–Pauling rule. With increase in V content, there is an increase in the total magnetic moment values.

Spin-polarized electronic structure calculations of Ti_2FeGa , $(\text{Ti}_{0.75}\text{V}_{0.25})_2\text{FeGa}$, TiVFeGa , and V_2FeGa alloys have shown that these alloys exhibit half-metallic behavior. Tetragonal $(\text{Ti}_{0.25}\text{V}_{0.75})_2\text{FeGa}$ alloy has a small band gap just below the Fermi energy level in the spin downward direction. It can be said that this tetragonal alloy exhibits only a half-metallic behavior. Second-order elastic constants and related elastic properties were calculated and evaluated for the first time. When Born stability conditions are taken into consideration, it is seen that all these alloys obey mechanical stability conditions. Equilibrium lattice constants, elastic constants and values obtained from bulk module (B), shear module (G), and Young module (E) confirm that the alloys are elastic and structurally stable. The studied alloys have a ductile nature, as it follows from the calculated B/G ratio, anisotropy, Pugh ratio, Poisson ratio, and Cauchy pressure. For Heusler alloys with a cubic crystal structure, with increasing V contribution, the ductility decreases, and for the alloys with tetragonal crystal structure, the ductility increases with increasing V contribution. From the Poisson's ratio calculated for these alloys, it was found that all the alloys have ionic character. All these alloys were determined to be anisotropic.

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