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The Theoretical Investigation on Electronic Behavior and Mechanical Properties of Ferromagnet Silver-Based Telluride: Ag_3FeTe_4

Ferromanyetik Gümüş-Tabanlı Tellürün Elektronik Davranışı ve Mekaniksel Özellikleri Üzerine Teorik Araştırma: Ag_3FeTe_4

Aytac Erkisi*[1], Bugra Yildiz[2]

[1]Pamukkale University, Faculty of Science and Letters, Department of Physics, Denizli, Turkey
[2]Hacettepe University, Faculty of Engineering, Department of Physics Engineering, Ankara, Turkey

Abstract

The magnetic nature, mechanical properties and electronic behavior of the ternary silver-based telluride system (Ag_3FeTe_4) which has sulvanite type simple cubic (SC) crystal structure which has 215 space number and conforms $P\bar{4}3m$ space group, have been inspected by spin-polarized Generalized Gradient Approach (GGA) under Density Functional Theory (DFT). First of all, to investigate suitable magnetic order for this system, it has been considered various antiferromagnetic phases which are A-type (A-AFM), G-type (G-AFM) and C-type (C-AFM) and ferromagnetic (FM) phase. As a result of calculations, it has been understood that, for Ag_3FeTe_4 compound, the energetically most favored magnetic phase is ferromagnetic. After that, well-optimized structural parameters and atomic positions have been obtained in ferromagnetic phase. The electronic band structure of this ferromagnetic system indicating half-metallic behavior due to the observed a small direct band gap (E_g = 0.297 eV) in spin-down states, has been investigated. Also, this compound has thermodynamic stability and structural synthesizability due to its calculated negative formation enthalpy values for all different types of magnetic phases. Also, the elastic constants provide the Born Huang criteria, the material is mechanically stable.

Keywords: Chalcogenide, Density functional theory, Electronic structure of bulk materials, Ferromagnet, Semiconductor

Öz

Sulvanit tipi basit kübik (BK) kristal yapıya sahip ve 215 boşluk sayısı ile $P\bar{4}3m$ uzay grubuna uyan üçlü gümüş bazlı tellür (Ag_3FeTe_4) sisteminin manyetik doğası, mekanik özellikleri ve elektronik davranışı, Yoğunluk Fonksiyonel Teorisi (YFT) altında spin-polarize Genelleştirilmiş Gradyan Yaklaşımı (GGY) ile araştırılmıştır. İlk olarak, bu sistem için uygun manyetik fazı araştırmak için, A-tipi, G-tipi ve C-tipi antiferromanyetik ve ferromanyetik faz düşünülmüştür. Hesaplamalar sonucunda, Ag_3FeTe_4 bileşiği için, enerjisel olarak en çok tercih edilen manyetik fazın ferromanyetik faz olduğu anlaşılmıştır. Daha sonra, iyi optimize edilmiş yapısal parametreler ve atomik pozisyonlar ferromanyetik faz için elde edilmiştir. Bu ferromanyetik sistemin, elektronik bant yapısında, spin-aşağı durumunda 0.297 eV'lik bir bant boşluğu gözlemlenmesi sebebiyle, yarı metalik bir davranış göstermektedir. Ayrıca, bu bileşik, tüm farklı tip manyetik fazlar için hesaplanan negatif oluşum entalpi değerleri nedeniyle termodinamik kararlılığa ve yapısal sentezlenebilirliğe sahiptir. Ek olarak, elastik sabitler Born Huang kriterlerini sağlaması sebebiyle mekanik olarak da kararlıdır.

Anahtar Kelimeler: Kalgojenit, Yoğunluk fonksiyonel teorisi, Yığın malzemelerin elektronik yapısı, Ferromanyetik, Yarı iletken

1. Introduction

Recently, transition metal chalcogenides have attracted the attention of many researchers, as their electronic nature is prone to half-metal or semiconductor properties and since they exhibit different magnetic behaviors and also, are usually very soft and flexible materials (Erkisi et al. 2019, Erkisi 2019, Nakamura, Kato et al. 2007, Nakamura, Akiyama et al. 2007, Nakamura et al. 2008, Zhou et al. 2016, Feng et al. 2013). In this view, the compounds consisting of transition metal group and chalcogenide group elements such as sulphur, selenium or tellurium element, have been used widely in technological fields such as solar cells and thermoelectric materials (Nakanishi et al. 1969, Miles et al. 2007, Skoug et al. 2010, Temple et al. 2012, Katagiri 2005), for a while. Therefore, there are many scientific researches

*Corresponding author: aerkisi@pau.edu.tr

Aytac Erkisi orcid.org/0000-0001-7995-7590
Bugra Yildiz orcid.org/0000-0002-0080-7096

about electronic, magnetic or thermal properties of these type of compounds in experimentally and theoretically (Nitsche et al. 1967, Zwick et al. 1999, Shannon et al. 2000, Doublet et al. 2000, Debus et al. 2002, Aiura et al. 2003, Klepp et al. 2000, Kars et al. 2005, Lu et al. 1993, Delgado et al. 2007). In recent years, especially ternary transition metal-based sulvanite type chalcogenide series having simple cubic (SC) crystal structure with 215 space number and conforming $P\bar{4}3m$ space group, have become the center of attention among material scientists (Pauling et al. 1932, Mujica et al. 1998).

In the early 2000s, using similar experimental methods, it was discovered that, some chalcogen-based compounds (Tate et al. 2008) and copper-based tantalate sulfide (Cu_3TaS_4) and selenide (Cu_3TaSe_4) exhibit p-type semiconductor properties by Tate (Newhouse et al. 2009). In some subsequent studies, the electronic and optical behaviors, of copper-based vanadate sulfide (Cu_3VS_4) investigated in experimentally by Lv et al., and it was discovered that this compound can be used in technology as a light absorbing material due to its suitable band gap (Lv et al. 2012), and after a short time, Ali et al. examined the electronic and optical characters, mechanical and thermal properties of copper-based sulfide series Cu_3TMS_4 (TM = V, Nb, and Ta) in computationally and they found that these compounds were found to be semiconductors (Ali et al. 20014). In some recent theoretical studies, by Erkisi et al., the electronic nature and some mechanical properties of some ferromagnetic copper-based (Erkisi, Surucu 2019) and zinc-based chalcogenides (Erkisi, Yildiz et al. 2019) investigated and the mentioned compounds were found to be half-metallic indicating to be able to used for spintronic applications in technology. In these two studies, due to the fact that there is a half-metallic electronic behavior in zinc-based chalcogenides as well as copper-based chalcogenides, in the present study, some silver-based chalcogenide compounds have been considered may exhibit interesting electronic behaviors, and therefore their electronic, magnetic and also some mechanical properties have been investigated.

In the present study, the electronic behavior in suitable magnetic nature and mechanical properties of new ternary silver-based ferrite telluride (Ag_3FeTe_4) which has simple cubic (SC) crystal structure with 215 space number and conforming to $P\bar{4}3m$ space group has been examined in detail. Therefore, firstly, four different magnetic orders, ferromagnetic (FM), A-type antiferromagnetic (A-AFM), G-type antiferromagnetic (G-AFM) and C-type antiferromagnetic (C-AFM), have been considered for this compound. The electronic band structure of this compound has been calculated for the stable magnetic order which is the ferromagnetic phase, by spin-polarizing within GGA. Adding a new material to the ternary chalcogenides family is of great importance, as the mentioned compound has a half-metallic behavior and therefore could be used in spintronic applications. To the best of our knowledge, the electronic behavior and stable magnetic phase of this material have not been examined yet in detail. The obtained results indicate that this telluride in the present study has half-metallic behavior in its stable ferromagnetic phase. In this view, the analysis of the electronic behavior and magnetic nature and also mechanical properties of this telluride system have been carried out from the first principles by using the VASP code. The computational details which are used in this study have been presented in the next section. The well optimized structural parameters, the suitable magnetic order and the calculated electronic band structure with the density of state (DOS) in the most stable magnetic phase, and some mechanical properties of this compound have been given in the third section. Conclusively, in the last section, the observed and obtained results have been concluded.

2. Material and Method

The density functional theory (DFT)-based calculations (Kohn et al. 1965; Hohenberg et al. 1964) in the present study, has been carried out by using VASP (Vienna Ab initio Simulation Package) (Kresse et al. 1993, 1996) code in which valence electron densities are expanded in plane-wave basis sets which determine the electronic states with the projector-augmented wave (PAW) method (Blöchl 994). The exchange-correlation effects have been described by Perdew, Burke and Ernzerhof (PBE) (Perdev et al. 1996) type pseudopotentials implementation of the generalized gradient approximation (GGA). In the mentioned ternary silver-based telluride, the electronic configurations of *Ag, Fe,* and *Te* atoms are as follows: $5s^14d^{10}$, $3d^74s^1$, and $4d^{10}5s^25p^4$.

For this composition, the well-optimized some structural parameters have been obtained by using automatically generated 12×12×12 Monkhorst-Pack scheme (Monkhorst et al. 1976) to perform the integrations in the irreducible Brillouin zone yielding 56 k-points. During this computational study, the plane-wave cutoff energy has been set to 900 eV. The atoms in primitive cell of this composition have been relaxed by using the quasi-Newton method and also, the convergence criteria for the force and energy have

been taken 10^{-8} eV/Å and 10^{-9} eV, respectively. per unit cell in the iterative solution of the Kohn-Sham equations. For the atoms in the primitive cell of the ternary silver-based telluride (Ag_3FeTe_4), the well-optimized atomic positions have been obtained by minimizing forces and pressures on this crystal system. After the optimization process of our system, to decide the most stable magnetic phase, a 2×2×2 super-cell containing 64 atoms has been produced and calculated energy-volume values for each different type of magnetic order. Then, the electronic behavior and some mechanical properties of this material have been examined in the most stable magnetic phase detected.

3. Results

The relaxed atomic positions in primitive cell for our system have been obtained by optimization process and then, the electronic and magnetic character of ternary silver-based telluride (Ag_3FeTe_4) having simple cubic (SC) sulvanite structure and conforming $P\bar{4}3m$ space group with 215 space number. The optimized atomic positions in the eight-atom primitive cell and three-dimensional (3D) crystal shape of the mentioned compound have been illustrated in Figure 1.

As seen from Figure 1 that, in the represented primitive cell, three silver atoms and one iron atom are positioned in 3d (0.5, 0, 0) and 1a (0, 0, 0) Wyckoff positions (Wyckoff 1963), respectively, while tellurium atoms are placed on 4e (0.237, 0.237, 0.237) positions. After the optimized structural parameters have been achieved, a 2×2×2 super-cell consisting of 64 atoms has been considered to detect the suitable magnetic order for our system. Finally, the electronic nature and mechanical properties of this telluride compound have been investigated in its energetically more favorable magnetic phase.

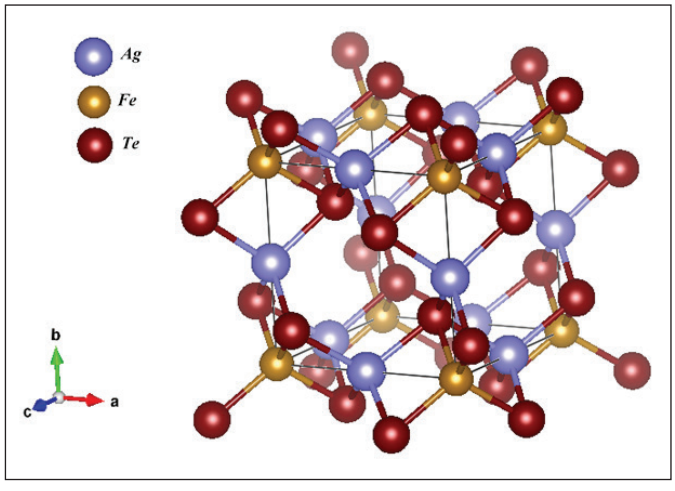

Figure 1: The 3D (three-dimensional) crystallographic shape of primitive cell with silver, iron and tellurium atoms.

3.1. The energetically Favorable Magnetic Phase and the Obtained Structural Parameters

A solid crystal having anyone of three different antiferromagnetic orders, consists of two ferromagnetic subsystems and each of which is mutually aligned and has large magnetization, but antiferromagnet material doesn't yield any magnetic field because its total magnetization is zero. It is well known that antiferromagnetic orders are three different types which are A-type, C-type and G-type. For each of these orders, the directions of the magnetic moments are organized in different types to be zero total magnetization (Han 2013), as shown schematically in Figure 2.

In order to detect the suitable magnetic order for this chalcogenide, the directions of the magnetic moments of the eight iron ions in the generated supercell have been regulated accordingly to the mentioned antiferromagnetic arrangements yielding zero total magnetization. Then, the formation enthalpy value (ΔH_f) which is usually calculated to decide the stability in thermodynamically or the synthesizability in structurally of a crystal, for each of different magnetic phases of this system, have been calculated by using the internal energy changes. It can be said that any solid crystal is structurally synthesizable and thermodynamically stable when the calculated formation enthalpy (ΔH_f) of it, is less than zero. For any solid crystal having its chemical formula A_xB_y, this energy value can be usually determined from the internal energy changes (Zhao et al. 2008) as given in Equation 1;

$$\Delta H_f = E_{tot} - (xE_A^{bulk} + yE_B^{bulk}) \quad (1)$$

where, E_A^{bulk} and E_B^{bulk} are the ground state energies of A and B atoms and E_{tot} is the total energy of the unit cell. Formation enthalpy can also be used to decide to be stable in which crystal structure or in which magnetic phase a compound which can be found in different crystal structures or different magnetic phases. In this respect, when the calculated enthalpy value of a solid crystal of its any structural or magnetic phase is less than that of others, it could be said that this magnetic phase or structure is energetically more suitable than others.

For different magnetic orders, as seen in Table 1, the calculated formation enthalpy values of this telluride system indicate that the suitable magnetic phase is ferromagnetic (FM) for this compound and also A-type AFM and

Table 1: The well-optimized bond lengths in primitive cell, lattice parameters and the calculated formation enthalpies of ternary silver-based telluride Ag_3FeTe_4 (*Space group: P$\bar{4}$3m, Space No:215*) for different magnetic orders.

Compound	a (Å)	d_{Fe-Te} (Å)	d_{Ag-Te} (Å)	ΔH_f (eV/f.u.)
Ag_3FeTe_4	6.432 (FM)	2.64249	2.74105	-0.321 (FM)
	6.434 (A-Type AFM)			-0.231 (A-Type AFM)
	6.371 (C-Type AFM)			0.369 (C-Type AFM)
	6.371 (G-Type AFM)			0.369 (G-Type AFM)

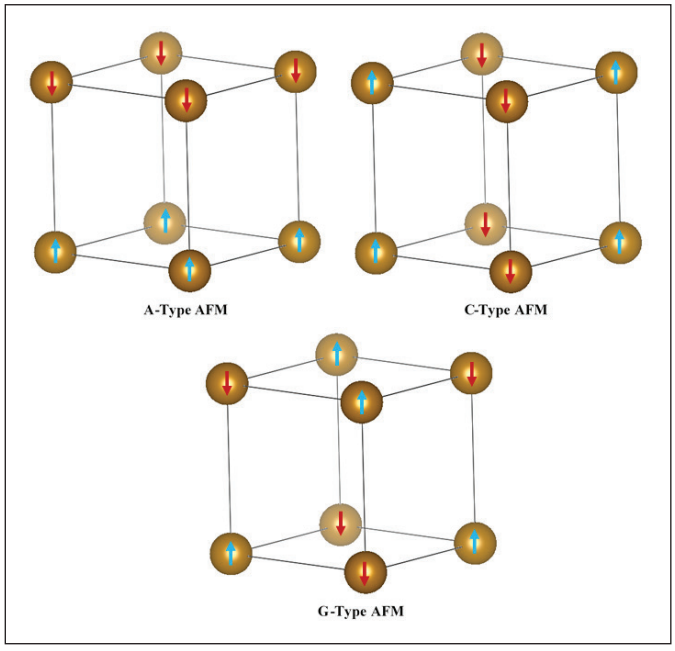

Figure 2. The schematic representation of different types of A-type, C-type and G-type antiferromagnetic orders for a simple cubic crystal.

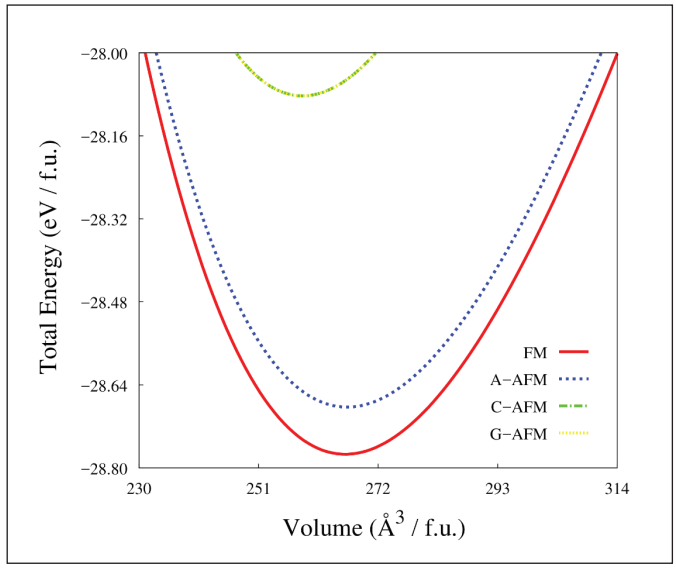

Figure 3. The energy-volume graphic of four different types of magnetic phases for ternary silver-based telluride (Ag_3FeTe_4).

ferromagnetic phase have thermodynamic stability and structural synthesizability, which is so important for the future possible technological applications, while C-type AFM and G-type AFM have no stability. Then, a well-optimized ground state energy-volume values of this system for each magnetic phase have been obtained and with the help of these values, it has been plotted as shown in Figure 3 by fitting the Vinet equation of state (Vinet et al. 1969). For this telluride system, a well-converged ground state has been achieved, maximum 1% asymptotic standard errors. For each magnetic phase, the obtained structural parameters have been presented in Table 1.

The graphed energy-volume plots for four different type magnetic orders, show that C-type and G-type antiferromagnetic orders for this compound are not suitable in energetically since our system has much higher ground state energies in these magnetic phases than the others. In the mentioned figure, it can be obviously understood that FM phase is most suitable for this compound due to have somewhat lower energy than A-type AFM phase and this is compatible with the formation enthalpies previously calculated for all magnetic phase types. To the best of our knowledge, to make any comparison, there is not detailed study or any investigation about this chalcogenide in literature yet. Furthermore, it can be said that the bond lengths between silver and tellurium atoms are greater than the bond lengths between iron and tellurium atoms in the primitive cell of ternary silver-based telluride.

3.2. The Electronic Nature of Ag_3FeTe_4 Telluride

The electronic nature of the ternary silver-based telluride has been understood from the electronic band structure and total density of state calculated by spin-polarizing with the GGA approach. The observed electronic band structure of

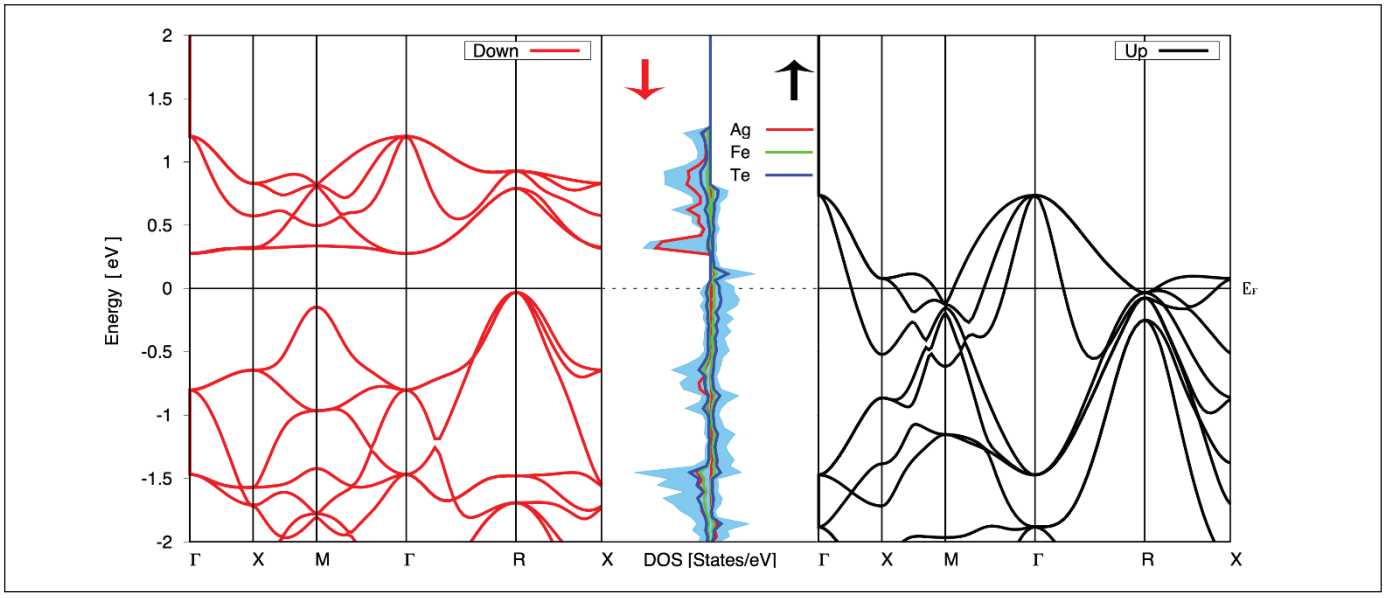

Figure 4: Spin-polarized energy band structure with the total density of electronic state (DOS) of ternary silver-based telluride (Ag_3FeTe_4) within GGA.

this chalcogenide system has been plotted along the high symmetry directions for both spin states in the Brillouin zone as demonstrated in Figure 4. As apparently shown in this figure, ternary silver-based telluride (Ag_3FeTe_4) having ferromagnetic nature, behaves as half-metallic material due to have a small indirect band gap (E_g = 0.297 eV and from R to Γ point) in spin-down state in observed its electronic band structure. In addition, the difference between spin-down and spin-up channels hint that this telluride system is not paramagnetic with regards to magnetic properties.

In order to see the orbital effects in the electronic band structure more clearly, the total and orbital projected partial density of electronic states for ternary silver-based telluride system (Ag_3FeTe_4) have been plotted as given in Figure 5. For this system, it can be obviously seen the dominancy of unfilled *p*-orbitals of tellurium (*Te*) namely chalcogen atoms for the valence band below Fermi level, while unfilled *3d* states of iron (*Fe*) atoms are dominant for the conduction band above Fermi level. In the region below Fermi level, approximately between -3 eV and 0 eV, it has been observed hybridizations in telluride system, between *d*-states of iron (*Fe*) and silver (*Ag*) atoms and *p*-orbitals of tellurium (*Te*) atoms. Furthermore, above the Fermi level almost between 0 eV and 1.5 eV, there is hybridizing between *p*-orbitals of tellurium (*Te*) atoms and *d*-orbitals of iron (*Fe*). In the same band, it is seen that the fully-filled *4d*-states of silver (*Ag*) atoms are not effective on the electronic structure. Moreover, it can be understood from Figure 5 that, *5s*-

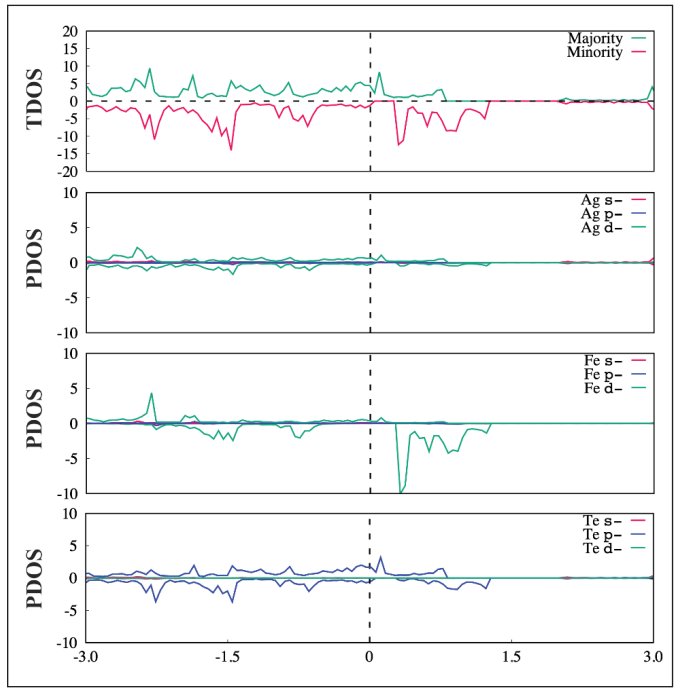

Figure 5: The observed orbital projected partial and total density of electronic states of atoms in Ag_3FeTe_4 compound.

and *4d*- states, which have very low density of states, of tellurium (*Te*) atoms in this compound haven't remarkable effect on chemical bonding features of ternary silver-based ferrite telluride system. Similarly, as seen from the related figure that, *s*- and *p*- orbitals of iron (*Fe*) and silver (*Ag*) atoms in this composition, as plotted with red and blue lines

respectively, haven't an important role in chemical bonding and the formation of related compound structure. On this subject, the electronic behavior of this telluride system could be determined by especially *d*-orbitals of iron (*Fe*) atoms which is a transition metal atom, and *p*-orbitals of tellurium (*Te*) atoms and hybridizations between them.

The total magnetic moments of ferromagnetic semi-metallic materials are expected to be close to the integer value, as a typical feature. The calculated total magnetic moment of this telluride compound is much close to the integer value in accordance with the mentioned feature of half-metallic materials ($\mu_{Ag_3FeTe_4} = 2.908\ \mu_B$). Moreover, the data obtained from the self-consistent calculations show that, the partial magnetic moments of the iron atoms (*Fe*) play an effective role on the total magnetic moment of this composition, as presented in Table 2. In this regard, it can be said that the iron atom (*Fe*) has responsibility for the ferromagnetic nature of this telluride system.

Table 2. The determined total magnetic moment (μ_B) of the silver-based Ag_3FeTe_4 telluride in ferromagnetic order and total magnetic moments of silver (*Ag*), iron (*Fe*) and tellurium (*Te*) atoms in this composition.

Material	μ_{tot} (μ_B)	μ_{atom} (μ_B)
Ag_3FeTe_4	2.908	μ_{Ag} = - 0.010
		μ_{Fe} = 2.954
		μ_{Te} = -0.035

3.3. The Predicted Mechanical Properties of Ag_3FeTe_4 Telluride

The stress-strain approach (Page et al. 2001) has been used under the *ab initio* method to calculate the elastic constants that can be used to study the mechanical stability of this telluride system and to determine some of its mechanical properties. C_{11}, C_{12} and C_{44} are three independent elastic constants (Mouhat et al. 2014), for a solid crystal having cubic symmetry. The second order elastic constants for ternary silver-based telluride (Ag_3FeTe_4) calculated under this approximation within the first principles methods have been presented in Table 3.

A solid crystal is expected to have mechanical stability, which is a desirable feature in industry and technology, and to resist external stresses. To be mechanically stable, the calculated elastic constants, have to satisfy Born-Huang criteria to understand the mechanical stability of a material (Mouhat et al. 2014). These conditions for any solid crystal having cubic symmetry are given in Eq. 2.

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

The determined second order elastic constants of this compound by using "stress-strain" method, of this compound show its mechanical stability due to satisfy the above-mentioned criteria.

The calculated C_{44} constant for a cubic crystal, gives information about resistance to shear deformation across the (100) plane in the [110] direction while the information about the resistance to shear deformation on the (110) plane in the $[1\bar{1}0]$ direction can be taken from the calculated (C_{11} - C_{11})/2 value (Knowles et al. 2015, Arıkan et al. 2014, Zener et al. 1948). It is clearly seen from the calculated constants as seen in Table 3 that, for silver-based Ag_3FeTe_4 telluride, resistance to shear deformation across the (100) plane in the [110] direction is higher than the resistance to shear deformation on the (110) plane in the $[1\bar{1}0]$ direction.

The idea of about a material's ductility can be obtained by using Cauchy pressure ($C_p = C_{12} - C_{44}$), which can be calculated with the help of elastic constants (Pettifor 1992). In this regard, if a crystalline Cauchy pressure is calculated as a positive value, the crystal can be considered as a ductile material, on the contrary, if this pressure value is negative, it can be considered as a fragile. In this computational study, the ternary silver-based telluride compound is ductile material since its calculated Cauchy pressure value is positive. It is an industrial desirable feature that a material is ductile. Because a fragile material does not have the ability to absorb energy and doesn't deform plastically, so that it tends easily under stress and strain (Mercier 2002).

3.3.1. Some Predicted Elastic Features by Using Elastic Constants

In this section of this research, technologically vital elastic

Table 3. The determined Cauchy pressure (C_p) and second order elastic constants of ternary silver-based telluride (Ag_3FeTe_4) under GGA approximation.

Compound	C_{11}(GPa)	C_{12}(GPa)	C_{44}(GPa)	C_p(GPa) = C_{12}-C_{44}
Ag_3FeTe_4	19.356	13.019	3.833	9.186

properties such as bulk moduli (B) and shear moduli (G), Young's modulus (E), Poisson's ratio (σ) and Pugh's ratio (B/G) have been predicted for our material ternary silver-based ferrite Ag_3FeTe_4 telluride, by employing formerly determined elastic constants in Section 3.3. The upper limit of bulk and shear moduli (B_V, G_V) have been estimated from Voigt (Voigt 1928) approximation, the lower limit of bulk and shear moduli (B_R, G_R) have been estimated from Reuss (Reuss 1929) approximation and finally average values of bulk and shear moduli (B_H, G_H) have been estimated from Hill (Hill 1952) approximation by using Eqs.3-6. Since, any solid crystal in cubic structure, lower and upper limit of bulk moduli is equal to each other as seen from the Eq. 3., only the average value of bulk moduli (B) has been added to Table 4.

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

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

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

$$B_H = (1/2)(B_V + B_R) \text{ and } G_H = (1/2)(G_V + G_R) \quad (6)$$

It is seen in Eq. 7 and Eq. 8, Young's modulus (E) and Poisson's ratio (σ), which could provide us vital information about the compressibility of a material, could be predicted as a function of formerly deduced bulk (B) and shear moduli (G) (Wu et al. 2014).

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

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

The estimated Young's moduli (E), which has been tabulated in Table 4, of ternary silver-based ferrite Ag_3FeTe_4 telluride demonstrate that the material could be treated as soft material. In addition to that, bulk (B) moduli, upper lower and average value of shear moduli (G_V, G_R and G_H), Poisson's ratios (σ) and Pugh's ratio (B/G) have been shown in Table 4, too.

If B/G ratio, of any solid crystal is higher than the critical value 1.75, material counted as ductile otherwise brittle (Pugh 1954). One could deduce from Table 4, in our case material is soft and ductile. In addition, this result is compatible with our expectation from Section 3.3 Cauchy pressure (C_p) predictions. Also, to visualize the mechanical properties better, two and three-dimensional (3D) predicted elastic properties of Ag_3FeTe_4 compound Young's moduli, linear, shear moduli and, Poisson's ratio have been drawn in Figure 6.

The estimated Poisson's ratio (σ), could be used for determining the compressibility or incompressibility of the material. If Poisson ratio value is around 0.5 material could be considered nearly incompressible, otherwise if the value is around 0.3 it can be considered nearly compressible (Gupta et al. 2017). As one can see from the Table 4, our value is around 0.4. Therefore, this indicates that our material cannot be considered as compressible or incompressible. Also, for any solid crystal, if Poisson's ratio is around 0.1 the bond is ionic, if around 0.25 is the bond is covalent, if it is higher than 0.25 the bond is metallic (Bannikov et al. 2007). Therefore, it is metallic bond for our case.

Another important mechanical parameter is shear anisotropy factor of the crystal. It presents vital knowledge about anisotropicity. Shear anisotropy factor of a cubic crystal, for the {100}, {010} and {001} planes are , is shown in Eq. 9 and for the {110} planes are , is shown in Eq. 10 as a function of elastic constants (Lau 1998).

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

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

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

Both shear anisotropy factor of ternary silver-based ferrite Ag_3FeTe_4 telluride have been presented in Table 5. If $2C_{44} = C_{11} - C_{12}$ the value of A goes to 1 and the material has isotropic nature. In our case, for both directions, the value is around 1 and it could be said that the material is isotropic. Also, this result is compatible with Figure 6, in which elastic modules symmetric for all axis.

3.3.2. The Predicted Some Thermal Properties

In this part of this study, some thermal features such as wave velocities (v_m, v_t and v_l), of ternary silver-based ferrite Ag_3FeTe_4 telluride, melting temperature (T_{Melt}) and

Table 4. The predicted bulk (B), shear (E) and Young's moduli (E), Poisson's (σ) and Pugh's ratios (B/G) of ternary silver-based ferrite Ag_3FeTe_4 telluride.

Compound	B (GPa)	G_V (GPa)	G_R (GPa)	G_H (GPa)	E (GPa)	B/G	σ
Ag_3FeTe_4	15.13	3.57	3.54	5.55	9.88	4.314	0.391

finally Debye temperature (θ_D) have been presented. The transverse and longitudinal sound wave velocities v_t and v_l of the material are predicted as a function of formerly determined shear (G) and bulk (B) moduli in Eq. 11 and 12 by using Navier's equation (Schreiber et al. 1973).

Table 5. The determined A and (anisotropy shear factors) of ternary silver-based ferrite Ag_3FeTe_4 telluride

Compound	A for the {100} planes	A_ for the {110} planes
Ag_3FeTe_4	1.188	1.135

$$v_t = [G / \rho]^{1/2} \quad (11)$$

$$v_l = [(B + (4G/3))/ \rho]^{1/2} \quad (12)$$

Then, v_t and v_l values are used to calculate the average sound wave velocity (v_m) in Eq. 13 (Anderson 1963):

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

All the estimated values of ternary silver-based ferrite Ag_3FeTe_4 telluride have been tabulated in Table 6. Other important the thermal feature of a material is the Debye

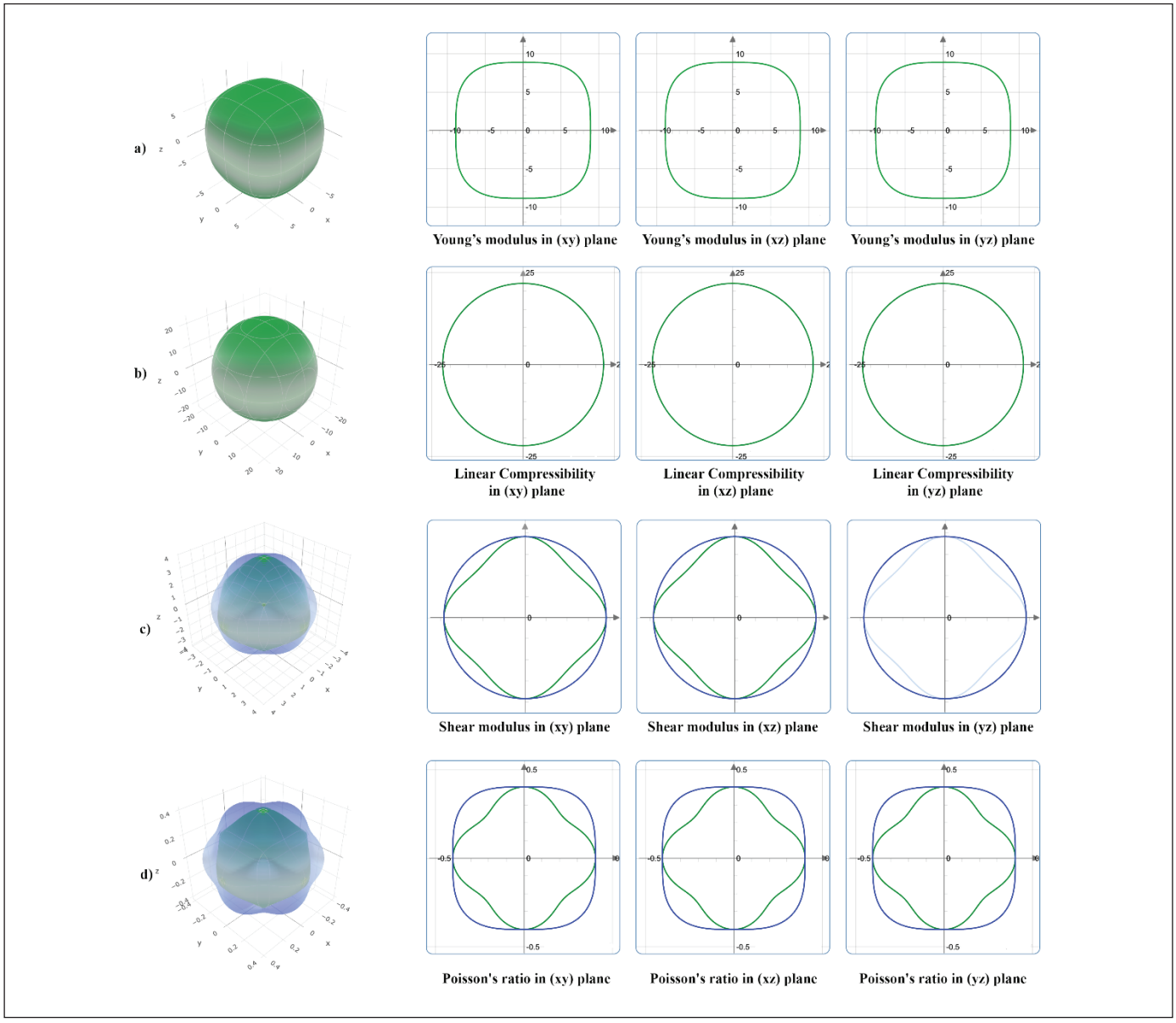

Figure 6. Two and three-dimensional (3D) predicted elastic properties of Ag_3FeTe_4 compound a) Young's moduli b) Linear Compressibility c) Shear moduli and d) Poisson's ratio (ELATE 2016).

Table 6. The determined transverse (v_t), longitudinal (v_l), and average (v_m) wave velocities and also Debye (θ_D) and melting temperatures (T_{Melt}) of ternary silver-based ferrite Ag_3FeTe_4 telluride.

Compound	v_t (m/s)	v_l (m/s)	v_m (m/s)	θ_D (K)	T_{Melt} (K)
Ag_3FeTe_4	1576	3251	1771	163.9	668 ± 300

temperature (θ_D). High Debye temperature could mean high melting temperature and high thermal conductivity. For this material, Debye temperature has been estimated by using Eq. 14 (Anderson 1963):

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

where k the Boltzmann's constant, N_A is the Avogadro's number, n is the number of atoms in the molecule, $\hbar$ is the Planck's constant, M is the molecular weight, ρ is the density of the material and finally v_m is the average sound wave velocity. The estimated Debye temperatures (θ_D) for ternary silver-based ferrite Ag_3FeTe_4 telluride has been presented in Table 6.

Lastly, the melting temperature has been roughly predicted for the crystal in this study by adopting the formerly calculated C_{11} elastic constant value in Table 3 (Fine et al. 1984).

$$T_{Melt} = \left[553\,K + \left(\frac{5.91\,K}{GPa}\right)C_{11}\right] \pm 300\,K \quad (15)$$

One could see from the Table 6, the approximately estimated melting temperatures for this telluride is consistent with the determined Debye temperatures.

4. Conclusion and Comment

In this research, for the most suitable magnetic order, mechanical properties and electronic features of new ternary silver-based ferrite Ag_3FeTe_4 telluride, which has 215 space number and conforms P43m space group, has been inspected in detail. The graphed volume-energy plot and determined negative formation enthalpy of this ternary silver-based ferrite telluride demonstrate that the crystal is ferromagnetic and synthesizable. With the half-metallic nature with small indirect band gap (E_g = 0.297 eV) in spin-down state of silver-based ferrite Ag_3FeTe_4 telluride, is a promising material for technological applications such as spintronic devices. Since the elastic constants provide the Born Huang criteria, the material is mechanically stable. Also, with the positive Cauchy pressures and high Pugh's ratio, the crystal is soft and has high ductility. In addition to that, the mentioned material is isotropic due to the value of shear anisotropy factor for all directions are around 1.

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