Ab initio investigation of the electronic structure, elastic and magnetic properties of quaternary Heusler alloy $Cu_2MnSn_{1-x}In_x$ ($x = 0, 0.25, 0.5, 0.75, 1$)

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Received 6 March 2019; accepted 28 March 2019

Structural, elastic, electronic and magnetic properties of the quaternary Heusler alloys $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) are calculated using the full-potential linearized augmented plane wave (FP-LAPW) method in the framework of the density functional theory (DFT) and implemented in WIEN2k code. The exchange-correlation potential is evaluated using the generalized gradient approximation (GGA) within the Perdew-Burke-Ernzerhof (PBE) parameterization. Our theoretically results provide predictions for the mixed $Cu_2MnSn_{1-x}In_x$ in which no experimental and theoretical data are currently available. The lattice parameter and bulk modulus as well the elastic constants and their related elastic moduli for $Cu_2MnSn_{1-x}In_x$ have been calculated. Also, the electronic properties including density of states and band structures indicate the metallic character for $Cu_2MnSn_{1-x}In_x$. Morever, this quaternary Heusler alloy is found to be ferromagnetic, brittle and anisotropic in nature.

Keywords: Ab-initio calculations; quaternary Heusler alloys; electronic structure; elastic and magnetic properties; ferromagnetic.

PACS: 63.20.Dj; 71.15.Mb; 62.50.+p

DOI: https://doi.org/10.31349/RevMexFis.65.468

1. Introduction

Recently, the discoveries of the giant magnetoresistance (GMR) and tunneling magnetoresistance (TMR) [1,2] opened the line of research called spintronics. Spintronics are composed of materials for which only one spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at the Fermi energy (E_F) [3]. Therefore, these materials utilize the spin in addition to the charge of electrons to carry the current. These remarkable materials, and their relatives (a vast collection of more than 3000 compounds) are today known as Heusler and half-Heusler compounds, have been discovered in 1903 when Friedrich Heusler had shown that Cu_2MnAl alloy behaves ferromagnetically even though none of its constituent elements are magnetic [4]. In 1983, de Groot *et. al.* [5] discovered half-metallic ferromagnetism in semi-Heusler compound NiMnSb by using first-principle calculation based on density functional theory. They first attracted interest of the magnetism community due to their high Curie temperatures [6] and being predicted to be half metallic ferromagnets [7]. In recent years, Heusler compounds are investigated due to their potential application in spintronics, green-energy-related fields, such as solar cells or thermoelectrics, superconductors [8], ferromagnetic shape memory alloys [9] and magnetic actuator [10].

Cu_2MnZ compounds have attracted much theoretical and experimental attention [11-13] for magneto-resistive device applications. The results, of Oxley *et al*. [14], are given of comprehensive measurements on the magnetic and crystallographic properties of the ferromagnetic Heusler alloys Cu_2MnZ (Z = Al, In, Sn, Ge, Sb, Bi and Ga), and they also discussed the indierct exchange effects which may give rise to ferromagnetism and antiferromagnetism in Heusler alloys. Dunlap *et. al.* [15] have studied the effects of rapid quenching on the structural and magnetic properties of the Heuler alloy Cu_2MnSn. Buschow *et. al*. [16] have studied the magneto-optical properties of metallic ferromagnetic materials Cu_2MnZ (Z = Al, Sn and In). Entel *et. al*. [17] computed the lattice parameters, magnetic moments, types of magnetic order and valence electron to atom ratios for series of Heusler compounds with the $L2_1$ structure, such as Cu_2MnZ (Z = Al, Ga and In). Hamri *et. al*. [18] illustrated that all the studied ferromagnetic systems X_2MnSn (X = Cu, Ni, Pd) exhibit a metallic character and possess an interesting elastic constants.

Besides ternary X_2YZ compounds, there exist also large assortments of substitutional quaternary alloys of the type $X_2Y_{1-x}Y'_xZ$, $(X_{1-x}X'_x)_2YZ$ and $X_2YZ_{1-x}Z'_x$. One of the substitutional series that attracted interest as potential material for magneto-electronics was $Co_2Cr_{1-x}Fe_xAl$ [19]. Drawback of these series is that it is hard to be stabilised in the $L2_1$ structure. Later, Seema *et. al*. [20] have investigated the effect of substitution of main group element on the electronic structure and magnetic properties of Co-based quaternary Heusler compounds $Co_2CrGa_{1-x}Ge_x$ ($x = 0-1$) using first-principles density functional theory. Paudel *et. al*. [21] have studied the mechanical stability and physical properties

of $Co_2V_{1-x}Zr_xGa$ ($x = 0$, 0.25, 0.50, 0.75, 1) by utilizing ab-initio calculations based on density functional theory within GGA-PBE, GGA+U and the quasi-harmonic Debye model.

Recently, Benichou *et. al.* [22] have investigated the structural, elastic, electronic and magnetic properties of quaternary Heusler alloy $Cu_2MnSi_{1-x}Al_x$ ($x = 0 - 1$) using a first-principles calculation by substituting the main group element (Si by Al) in this compound. The $Cu_2MnSi_{1-x}Al_x$ alloy is found to be ferromagnetic, metallic compound and has a ductile behavior. In this paper, we systematically study the effect of alloying Cu_2MnSn full Heusler alloy with In, namely, $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) alloy. To the best of our knowledge, there are no experimental and theoretical works exploring $Cu_2MnSn_{1-x}In_x$ quaternary alloy. The study was based on a full-potential augmented plane wave method within the framework of density functional theory.

The remainder of this paper is arranged as follows : In Sec. 2, we give with a brief description of the method used and details of the calculations. Section 3 deals with the crystal structural aspects. In Sec. 4, the structural parameters, elastic constants, magnetic and the electronic properties, for the full-Heusler compounds of the type Cu_2MnZ, where Z stands for Sn and In, and their quaternary alloy $Cu_2MnSn_{1-x}In_x$ ($x = 0.25, 0.5, 0.75$), are presented and analyzed. Finally, conclusions are summarized in the last section. The present calculations provide predictions and may serve for a reference.

2. Computational details

In the present study, the first principles calculations are performed within the full potential linearized augmented plane wave (FP-LAPW) method [23] as implemented in the WIEN2k code [24], based on the density functional theory (DFT) [25,26]. The exchange and correlation potential was calculated using the generalized gradient approximation [27]. The plane wave parameter $R_{MT} \times K_{\max}$ was 7.0, and to ensure the correctness of the calculations, we have taken $l_{\max} = 10$. The $G_{\max}$ parameter was taken to be 12.0. The separation energy between the core and the valence states has chosen as -7.0 Ry. Thus, the atomic sphere radii were set to 2.2, 2.0, 2.0 and 2.5 $a.u.$ (atomic unit) for Cu, Mn, Sn and In atoms, respectively. The number of k-points used in the irreducible part of the Brillouin Zone are 286 and 4 for ternary and quaternary alloys respectively, which give convergence of 10^{-4} Ry in the total energy.

3. Crystal Structure

Full-Heusler alloys are represented by the generic formula X_2YZ, where X and Y denote transition metals and Z is an $s - p$ element. The atomic positions described with the Wyckoff coordinates for X (Cu) atoms are (1/4,1/4,1/4), (3/4,3/4,3/4), while (1/2,1/2,1/2) for Y (Mn) and for Z (Sn, In) it is (0,0,0). In Fig. 1, we show the crystal structure of $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) alloys, where the present structures composed of four interpenetrating face-centered-cubic (fcc) sublattices, with $L2_1$ phase and $Fm - 3m$, space group no. 225. To simulate Cu_2MnSn_{1-x}

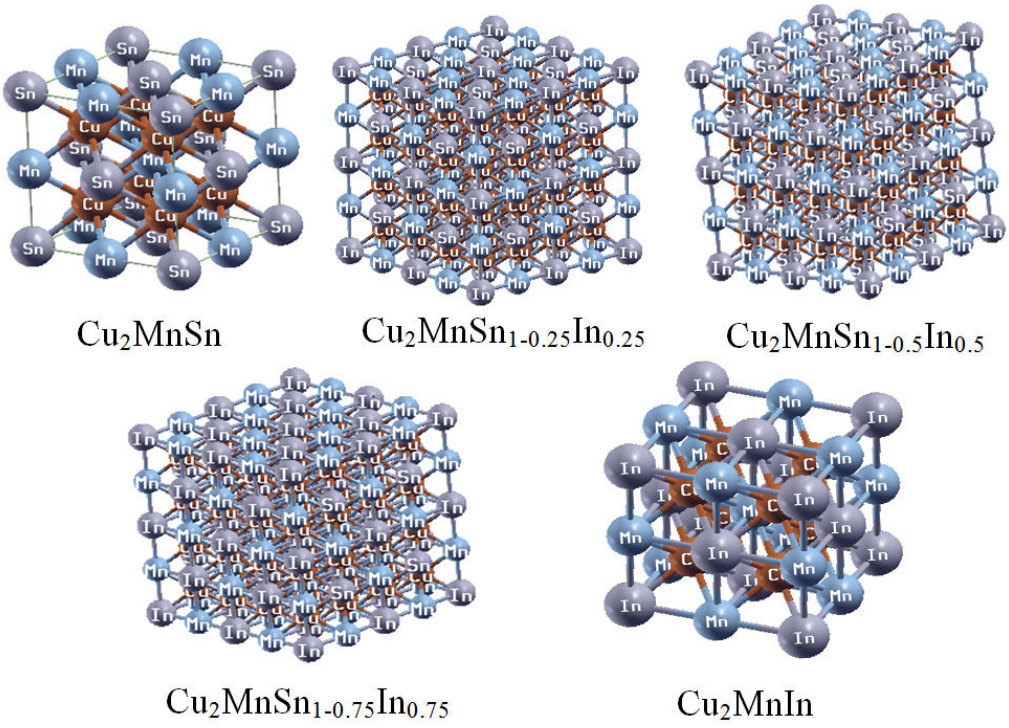

FIGURE 1. Crystal structure of the $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) alloys obtained with XCrysDen.

TABLE I. Calculated lattice parameter (a), bulk modulus (B), its pressure derivative (B'), and equilibrium energy for the $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75, 1) Heusler alloy.

Compounds	a_0 (Å)	B (GPa)	B'	E_{FM} (Ry)
Cu_2MnSn	6.2432	100.9400	4.8760	-21295.589815
	6.24 [18]	105.33 [18]		
	6.2337 [30]	101.31 [30]		
	6.26 [Theo,31]			
	6.17 [Exp,32]			
	6.168 [16]			
	6.1674 [17]			
	6.173 [Exp,14]			
$Cu_2MnSn_{1-0.25}In_{0.25}$	6.22075	103.0271	3.0794	-169180.697401
$Cu_2MnSn_{1-0.5}In_{0.5}$	6.21615	109.5466	2.9170	-167997.563381
$Cu_2MnSn_{1-0.75}In_{0.75}$	6.202	113.0188	4.4334	-166814.419381
Cu_2MnIn	6.1957	107.8258	4.1911	-20703.994345
	6.2021 [Theo,30]	106.96 [Theo,30]		
	6.206 [16]			
	6.206 [Exp,14]			

Al_x quaternary alloys, we consider a ($2 \times 2 \times 2$) supercell eight times greater than $L2_1$ unit cell. The supercell is then constituted of 32 atoms; 16 Cu, 8 Mn and 8 Sn/In, as shown in Fig. 1. The Sn atoms are replaced by In atoms to simulate different concentrations. Replacement of 2, 4, 6 and 8 number of those eight Sn atoms by In atoms leads to $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75, 1) respectively.

4. Results and discussion

4.1. Structural properties

The equilibrium lattice constants, bulk modulus and their first pressure derivatives, which are quoted in Table I, are fitting by the computed total energies to the empirical Murnaghan's equation of state [28]. We have done structural optimization of $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75) Heusler alloys by using nonmagnetic (NM) and ferromagnetic (FM) states. The plot of total energy variation versus volume under both non-magnetic and ferromagnetic phases with different concentrations is shown in Fig. 2. Clearly FM state is favorable in energy than the corresponding NM state. The optimized lattice constants for Cu_2MnSn and Cu_2MnIn alloys, which are also given in Table I, are in fairly good accordance with available experimental data [14,19] and previous theoretical calculations [16-18]. The maximal error for lattice parameters is less than 1.0%. To the best of our knowledge, there are no comparable studies about $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75) in literature, so we estimated the lattice parameters, for the selected concentrations 0.25, 0.5 and 0.75 by using the Vegard's law [29] in Eq. (1).

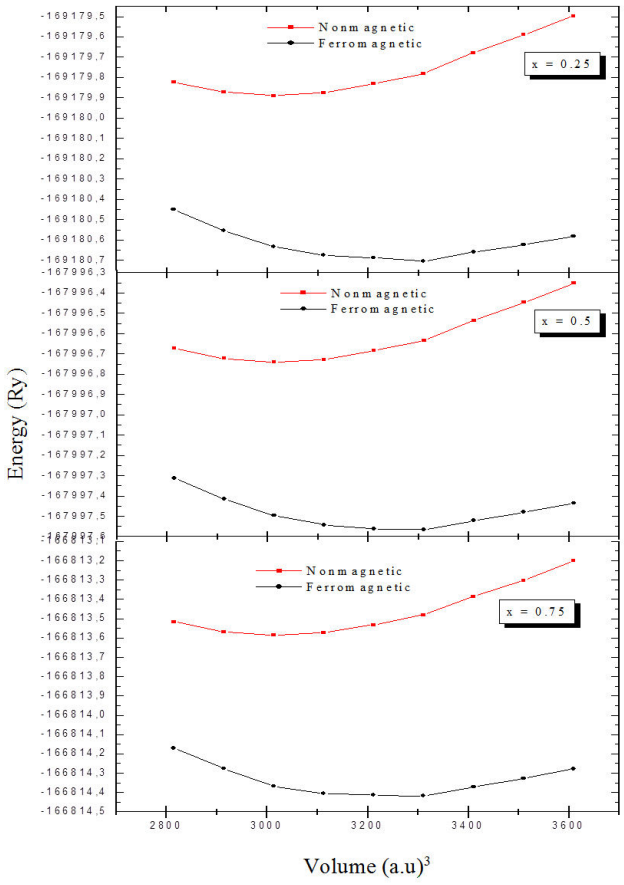

FIGURE 2. The total energy as a function of volume of $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75) quaternary Heusler alloys for nonmagnetic (NM) and ferromagnetic (FM) states.

$$Cu_2MnSn_{1-x}In_x : a(\text{Å}) = 6.24(1-x) + 6.19x \quad (1)$$

$$Cu_2MnSn_{1-0.25}In_{0.25} : a(\text{Å}) = 6.2275$$

$$Cu_2MnSn_{1-0.5}In_{0.5} : a(\text{Å}) = 6.215$$

$$Cu_2MnSn_{1-0.75}In_{0.75} : a(\text{Å}) = 6.2025$$

4.2. Elastic properties

We now discuss the mechanical properties of the parent compounds Cu_2MnSn, Cu_2Mnln and $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$, 0.5, 0.75) quaternary alloy, in order to confirm their mechanical stability in a cubic structure via calculation of the elastic constants (C_{ij}). These constants are fundamental and indispensable for describing the mechanical properties of materials because they are closely related to various fundamental solid-state phenomena, such as the stuctural stability, the bonding character between adjacent atomic planes and anisotropic character. The elastic constants require knowledge of the derivative of the energy as a function of lattice strain. In the case of cubic system, there are only three independent elastic constants, namely, C_{11}, C_{12} and C_{44}. The traditional mechanical stability conditions for a cubic stucture, which are known as the Born Huang criteria [33], are defined as follows: $C_{11} - C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$ and $C_{12} < B < C_{11}$. The obtainted elastic constants C_{ij}, summarized in Table II, are calculated by using a numerical first-principles method within GGA approximation in the WIEN2k package. The bulk modulus calculated from the theoretical values of the elastic constants $B = (1/3)(C_{11} + 2C_{12})$ are listed in Table II too, and it has nearly the same values as the ones obtained from energy minimization. As seen from Table II, the computed elastic constants of $Cu_2MnSn_{1-x}In_x$ for all compositions are positive and satisfy the above mechanical stability criteria indicating that the structures under study are elastically stable phases. The obtained results for Cu_2MnSn and Cu_2MnIn alloys agree quite well with earlier ab-initio calculation in Ref. [18] and that of Ref. [30] respectively. Within best of knowledge, there is no report on the experimental and theoretical elastic constants on the quaternary alloy. Therefore, our results are considered as purely predictive.

Besides this, we have also calculated various combinations of elastic moduli such as, Voigt's shear (G_V), Reuss's shear (G_R), Shear modulus (G), Young's modulus (E), Poisson's ratio (V), anistropy factor (A) and Kleinman parameter (ξ), which are listed in Table II, using the following equations [34-36]:

$$\text{Voigt's shear modulus} : G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (2)$$

$$\text{Reuss's shear modulus} : G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \quad (3)$$

$$\text{Isotropic shear modulus} : G = \frac{G_R + G_V}{2} \quad (4)$$

$$\text{Young's modulus} : E = \frac{9BG}{3B + G} \quad (5)$$

$$\text{Poisson's ratio} : v = \frac{3B - 2G}{2(3B + G)} \quad (6)$$

$$\text{Zener Anisotropy factor} : A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (7)$$

$$\text{Kleinman parameter} : \xi = \frac{C_{11} + 8C_{12}}{7C_{11} + 2C_{12}} \quad (8)$$

where G is the shear modulus, G_V is Voigt's shear modulus corresponding to the upper bound of G values and G_R is Reuss's shear modulus corresponding to the lower bound of G values.

In order to predict the brittle and ductile behavior of materials, Pugh [37] proposed an approximate criterion by the ratio B/G. Higher (lower) B/G ratio corresponds to ductile (brittle) behavior, and the critical value that separates brittle and ductile materials is about 1.75. The calculated values, listed in Table II, indicate that the B/G ratios are 2.766 and 3.125 for Cu_2MnSn and Cu_2MnIn respectively, suggesting the ductile nature of the parent ternary alloys, but for

TABLE II. Calculated elastic constants (in GPa), and elastic moduli B (in GPa), G (in GPa), B/G, E (in GPa), v, A, ξ for $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25 0.5, 0.75, 1).

Compounds	C_{11}	C_{12}	C_{44}	B	G	B/G	E	v	A	ξ
Cu_2MnSn	118.654	95.908	65.330	103.319	37.344	2.766	99.987	0.338	5.74	0.866
	102.03 [18]	91.71 [18]	66.81[18]							
	105.93 [30]	99.00 [30]	64.75 [30]							
$Cu_2MnSn_{1-0.25}In_{0.25}$	244.905	48.936	191.087	114.085	146.153	0.780	307.254	0.051	1.95	0.351
$Cu_2MnSn_{1-0.5}In_{0.5}$	319.038	14.453	220.733	115.666	190.228	0.608	368.609	0.031	1.44	0.192
$Cu_2MnSn_{1-0.75}In_{0.75}$	261.499	91.386	131.115	147.994	110.231	1.342	264.920	0.201	1.54	0.493
Cu_2MnIn	121.635	101.562	74.228	108.489	34.705	3.125	94.084	0.355	7.39	0.885
	114.45 [30]	103.22[30]	78.26 [30]							

TABLE III. Calculated values of total and partial spin magnetic moments (in μ_B) of $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1).

Compounds	M^{Cu}	M^{Mn}	M^{Sn}	M^{In}	$M^{interstitial}$	M^{total}
Cu_2MnSn	0.040	3.507	0.00004	—-	0.327	3.914
	0.03 [18]	3.73 [18]				3.93 [18]
						4.11 [Exp,39]
	0.04 [Theo,40]	3.79 [Theo,40]				3.81 [Theo,40]
						3.89 [17]
$Cu_2MnSn_{1-0.25}In_{0.25}$	0.057	3.529	0.001	-0.030	0.375	4.012
$Cu_2MnSn_{1-0.5}In_{0.5}$	0.053	3.500	0.002	-0.039	0.344	3.933
$Cu_2MnSn_{1-0.75}In_{0.75}$	0.030	3.426	0.003	-0.053	0.279	3.726
Cu_2MnIn	0.037	3.490	——-	-0.052	0.245	3.757
						3.7879[Theo,30]

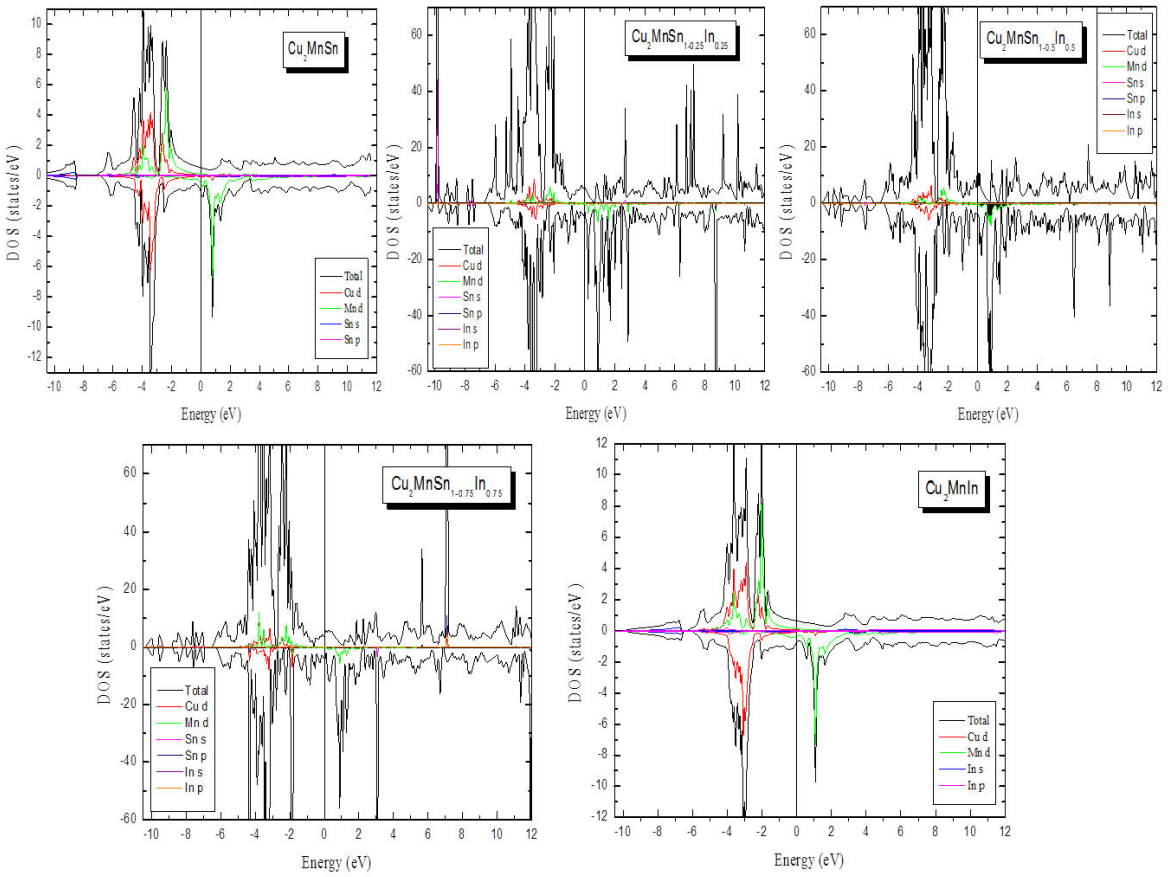

FIGURE 3. Total and partial density of states for $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) Heusler alloy. The verticale lines indicate the position of the Fermi level (E_F).

$Cu_2MnSn_{1-x}In_x$ quaternary alloys, the values of B/G ratio are between 0.608 and 1.342 indicating their brittle nature.

The Young's modulus (E) characterizes the stiffness of a material. The higher value of E, stiffer is the material. It can be seen, from Table II, that Cu_2MnSn is stiffer than Cu_2MnIn, and $Cu_2MnSn_{1-x}In_x$ quaternary alloy is also stiffer for the concentration $x = 0.5$ than $x = 0.25$ and 0.75. We also note that this quaternary alloy has a high Young's modulus, what classifies the studied compound as a strong incompressible material. The value of Poisson's ratio (v) is indicative of the degree of directionality of the covalent bonds. Its value for covalent materials is small ($v < 0.1$),

whereas the typical value for ionic materials is 0.25. Our calculated Poisson's ratios vary from 0.201 to 0.355, so the contribution in the intra-atomic bonding for Cu_2MnSn, Cu_2MnIn and $Cu_2MnSn_{1-0.75}In_{0.75}$ alloys is ionic, whereas for $Cu_2MnSn_{1-x}In_x$ ($x = 0.25$ and 0.5), v is less than 0.1 suggesting a covalent material. Elastic anisotropy factor (A) is equal to one for completely isotropic nature, while any different value shows anisotropy. The magnitude of the deviation from 1 is the measure of the degree of elastic anisotropy of the crystal. The calculated values of A factor shows that $Cu_2MnSn_{1-x}In_x$ alloy is anisotropic by nature. It is seen from the Table II that all the herein materials are anisotropic in nature but both the parent ternary compounds are more anisotropic than their quaternary alloy.

4.3. Electronic properties

Here, we study our results of electronic properties of $Cu_2MnSn_{1-x}In_x$ alloys by calculating the density of states (DOS) which is important for understanding the bonding properties. Therefore, the total (TDOS) and partial (PDOS) densities of states for spin-up and spin-down, using the GGA approximation, are calculated and depicted in Fig. 3. It is clear from Fig. 3 that both majority (up) and minority (down) spin band structures of $Cu_2MnSn_{1-x}In_x$ are strongly metallic. As seen from Fig. 3, there are two distinct regions in the spin-up and spin-down states of DOS of the parent Heusler alloys. The lowest valence bands below -8 eV for Cu_2MnSn (below -6 eV for Cu_2MnIn) are formed entirely from the s-states of Sn/In, while the bands from -6 to 4 eV for both Cu_2MnSn and Cu_2MnIn are principally caused by the Cu and Mn $3d$-states. Our results for Cu_2MnSn are in quite good agreement with earlier ab-initio calculations [18]. Morever, for $Cu_2MnSn_{1-x}In_x$ quaternary alloy, the mainly parts of the total densities of states localized around -4 to 3 eV are chiefly governed by the $3d$-states of Cu/Mn atoms.

4.4. Magnetic properties

The calculated total and local spin magnetic moments for $Cu_2MnSn_{1-x}In_x$ quaternary Heusler alloys are reported in Table III. It is clear from this table that our predictive results show that the total magnetic moments, which include the contribution from the interstitial region, comes mainly from the Mn atom, while the Sn, In and Cu atoms have a very small moment. Actually in Ni_2MnZ and Cu_2MnZ alloys, the magnetic moment can not be substantial larger than the magnetic moment on Mn atoms because only Mn determined the magnetic behavior of these alloys [38]. Morever, in case of ternary parent Cu_2MnSn and Cu_2MnIn full-Heusler alloys, the calculated value of spin magnetic moments 3.91483 and 3.75798 respectively, are listed in Table III which are close to earlier obtained theoretical data [30,14] and experimental result by Webster *et al.*, [39] which are also reported in Table III. The local spin magnetic moment on the non-transition metal atoms Sn (In) is small and aligned parallel (anti-parallel) to that of the Cu and Mn atoms. As far as we are aware, there are no reports on the magnetic moments for the quaternary alloy.

5. Conclusion

In summary, we have extensively investigated the structural parameters, elastic and mechanical, electronic and magnetic properties of the $Cu_2MnSn_{1-x}In_x$ quaternary alloy by utilizing first-principle calculations based on density functional theory within GGA-PBE. The optimized lattice parameters and spin magnetic moments for the parent full-Heusler alloys Cu_2MnSn and Cu_2MnIn were in qualitative agreement with the available experimental and theoretical data. Also, our predicted lattice constants of the quaternary alloy, in the stable magnetic configuration, exhibit a high tendancy with the estimated values by Vegard's law. The spin resolved density of states revealed that all the herein studied compounds have a perfect ferromagnetic and metallic character. The magnetic properties show that for these ferromagnetic compounds, the partial moment of In being antiparallel to the Cu, Mn and Sn atoms. The Mn atom is responsible for large magnetic moment in case of the ternary and quaternary Heusler alloys under study. Furthermore, according to mechanical stability conditions, our obtained elastic constants indicate that the $Cu_2MnSn_{1-x}In_x$ quaternary Heusler alloy is mechanically stable, anisotropic and has a brittle behavior. Most of the studied properties for $Cu_2MnSn_{1-x}In_x$ ($x = 0$, 0.25, 0.5, 0.75, 1) Heusler alloys, reported in this work, have not previously been established experimentally or theoretically. Finally, we hope that our results could provide baseline data for future investigations.

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