STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF Cu_2MnZ(Z=Al, Ga, In, Si, Ge, Sn, Sb): A FIRST-PRINCIPLES STUDY

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Abstract: *The structural, elastic, electronic and phonon properties of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) are investigated by first-principles calculations based on density functional theory. In this approach the local-density approximation (LDA) and generalized gradient approximation (GGA) are used for the exchange-correlation (XC) potential. The calculated lattice constant, bulk modulus, and elastic constants are in agreement with the previous ab-initio calculations and available experimental results. Electronic properties are discussed from the calculations of band structure and density of states. The direct method is used to derive the phonon frequencies and density of states.*

Keywords: HEUSLER ALLOY, ELECTRONIC BAND STRUCTURE, ELASTIC CONSTANTS, PHONON

1. Introduction

Heusler alloys have received much study due to their potential as key materials for spintronic devices [1-5]. Heusler compounds belong to a group of ternary intermetallics with the stoichiometric composition, X_2YZ, ordered in $L2_1$-type structure (space group Fm-3m) and many of these compounds are ferromagnetic. Full-Heusler alloys X_2YZ crystallize in the $L2_1$ structure. The unit cell consists of four interpenetrating fcc sublattices with the positions (0,0,0) and (0.5,0.5,0.5) for X, (0.25,0.25,0.25) for Y and (0.75,0.75,0.75) for Z atom. For Cu_2MnAl, the electronic, optical, elastic and magnetic properties were studied by Rai et al. [6] using the full potential linearized augmented plane wave method with the generalized gradient approximation (FPLAPW-GGA). They found that Cu_2MnAl is a ferromagnet metallic compound. In this work, we have aimed at to provide some additional information to the exhibit data on the structural, elastic, electronic and phonon properties of Cu_2MnZ(Z=Al, Ga, In, Si, Ge, Sn, Sb) alloys. The full phonon-dispersion curves are necessary for a microscopic understanding of the lattice dynamics. Knowledge of the phonon spectrum plays a significant role in determining various material properties, such as phase transition, thermodynamic stability, transport and thermal properties.

2. Computational Methods

The calculations were performed within the density functional theory, as implemented in the MedeA-Vasp package [7, 8]. In order to ensure the reliability of the calculations, the total energy and lattice parameter of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) alloys were calculated with respect to plane wave cutoff energy E_{cut} and k-point sampling. The optimization of the structural parameters is performed until the forces on the atoms are less than 0.02 eV/Å. The elastic properties (*G*, *E*) were calculated from the Hill value, which is a geometric mean of the Voigt and Reuss values [9]. The phonon dispersion curves of the considered materials have been calculated through the direct method [10], in which the forces are calculated via the Hellmann-Feynman (HF) theorem.

3. Results and Discussion

In Table 1, we summarize our calculated convergence parameters (E_{cut} and k-point), equilibrium lattice constant (a_0) Bulk modulus (*B*) and total magnetic moments (Mt) of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) compared with the available data in the literature. There is a good agreement between our results and that previously reported [6].

Table 1: *Calculated convergence parameters (Ecut, k-point), lattice constants (a_o), Bulk modulus (B) and total magnetic moments (Mt) for Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) alloys.*

		E_{cut}(eV)	k-point	a_0 (Å)	*B* (GPa)	M_t(μB)
GGA-PBE	Cu_2MnAl	376,696	7x7x7	5,928606 5,957[6]	124,24 115,64 [6]	3,5764 3,568 [6]
	Cu_2MnSi	344,196	8x8x8	5,864956	133,60	3,7303
	Cu_2MnGe	395,823	9x9x9	6,005586	114,80	3,9944
	Cu_2MnGa	344,196	5x5x5	5,956234	121,19	3,6176
	Cu_2MnSn	360,446	7x7x7	6,233775	101,31	3,8685
	Cu_2MnSb	360,537	6x6x6	6,313866	96,50	3,9057
	Cu_2MnIn	344,196	6x6x6	6,202166	106,96	3,7879
LDA	Cu_2MnAl	376,696	6x6x6	5,755385	153,49	3,2020
	Cu_2Mn Si	340,446	7x7x7	5,677539	170,76	3,3961
	Cu_2MnGe	361,492	6x6x6	5,815464	147,32	3,6596
	Cu_2MnGa	360,446	6x6x6	5,761216	164,45	3,3771
	Cu_2MnSn	344,196	7x7x7	6,038436	139,36	3,6249
	Cu_2MnSb	360,446	6x6x6	6,102149	125,51	3,6367
	Cu_2MnIn	360,537	5x5x5	6,002546	139,22	3,5131

Table 2: *The calculated elastic constants Cij (in GPa), shear moduli (in GPa) and Young's modulus (in GPa).*

		C_{11}	C_{12}	C_{44}	*G*	*E*
GGA-PBE	Cu_2MnAl	137.2 137.68 [6]	117.75 104.614 [6]	105.28 460.41 [6]	67.06 116.04 [6]	170.50
	Cu_2MnSi	128.33	136.24	89.43	52.08	138.27
	Cu_2MnGe	110.64	116.88	65.72	38.18	103.12
	Cu_2MnGa	124.49	119.55	90.00	54.99	143.30
	Cu_2MnSn	105.93	99.00	64.75	40.24	106.60
	Cu_2MnSb	80.38	104.56	29.27	12.73	36.58
	Cu_2MnIn	114.45	103.22	78.26	49.20	127.98
LDA	Cu_2MnAl	170.13	145.17	129.76	82.85	210.65
	Cu_2Mn Si	162.48	174.90	105.41	60.76	162.95
	Cu_2MnGe	137.52	152.22	85.38	48.29	130.59
	Cu_2MnGa	169.35	162.01	117.77	72.13	188.79
	Cu_2MnSn	142.35	137.86	83.84	51.20	136.85
	Cu_2MnSb	103.65	136.43	46.87	21.56	61.18
	Cu_2MnIn	149.53	134.06	100.69	63.51	165.38

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 well-known Born stability criteria are a set of conditions on the elastic constants (C_{ij}) that are related to the second-order change in the internal energy of a crystal under deformation. Cu_2MnZ(Z=Al, Ga, Sn, In) all fulfill the stability criteria, while the unstable Cu_2MnZ(Z= Si, Ge, Sb) fails to satisfy the Born criterion.

The electronic structure plays an important role in determining

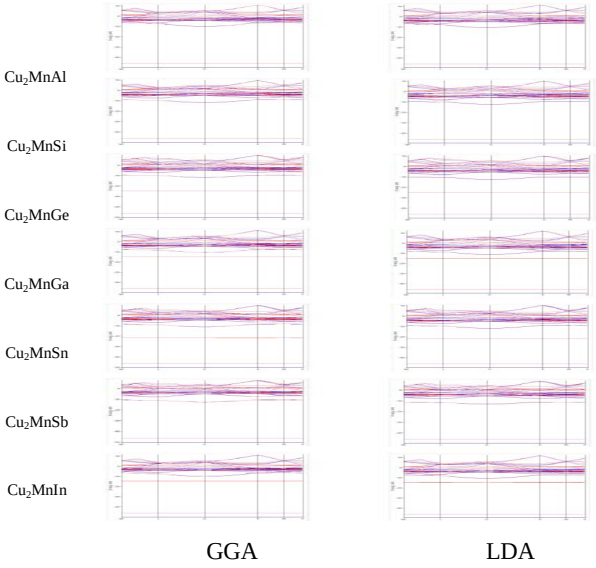

Fig. 1 *The spin resolved electronic band structure of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In). Solid red and blue lines are corresponding to spin up and down states, respectively.*

the magnetic properties of Heusler compounds. Fig. 1 shows the electronic structure of the Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In). Band structure calculations, which were performed using various methods (GGA, LDA) show almost the same shape. There is no gap between the two spin density of states at the Fermi level, meaning that it exhibits a typical metallic nature.

Fig. 2 shows the phonon dispersion curves along the high-

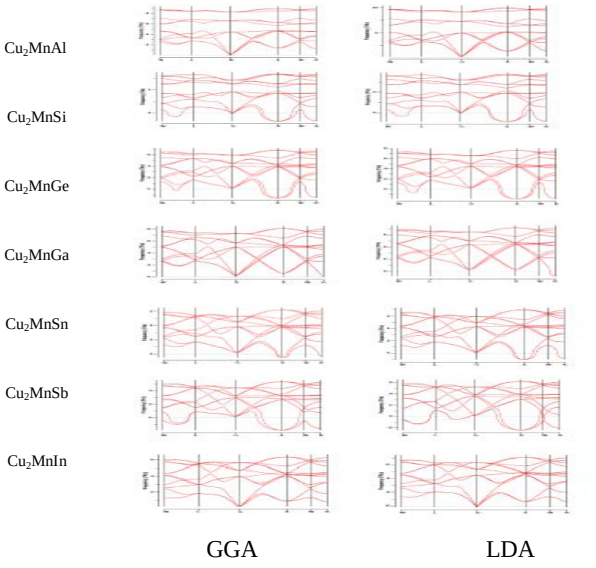

Fig. 2 *Calculated phonon dispersions of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In).*

symmetry directions for Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In). The calculated phonon dispersion curves of Cu_2MnAl and Cu_2MnIn confirm that these two compounds are dynamically stable in the $L2_1$-type structure without any imaginary phonon frequencies.

4. Conclusion

Structural, elastic, electronic and phonon properties for a series of Cu containing bulk Heusler alloys Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) were investigated by first-principles investigations. The lattice constant has been calculated using two different methods GGA and LDA and gave excellent agreement with others. The band structure for the Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) alloys were analysed and compared. The phonon properties of Cu_2MnZ(Z=Al, Si, Ge, Ga, Sn, Sb, In) were studied in the direct method.

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