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Ab initio study of the structural, electronic, elastic and magnetic properties of Cu_2GdIn, Ag_2GdIn and Au_2GdIn

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ABSTRACT

We preformed first-principle calculations for the structural, electronic, elastic and magnetic properties of Cu_2GdIn, Ag_2GdIn and Au_2GdIn using the full-potential linearized augmented plane wave (FP-LAPW) scheme within the generalized gradient approximation by Wu and Cohen (GGA-WC), GGA+U, the local spin density approximation (LSDA) and LSDA+U. The lattice parameters, the bulk modulus and its pressure derivative and the elastic constants were determined. Also, we present the band structures and the densities of states. The electronic structures of the ferromagnetic configuration for Heusler compounds (X_2GdIn) have a metallic character. The magnetic moments were mostly contributed by the rare-earth Gd 4f ion.

1. Introduction

Heusler compounds are ternary intermetallic compounds that have the general composition X_2YZ. In this class, X and Y represent d-electron transition metals, and Z denotes an sp-electron element [1]. In recent years, Heusler compounds have been extensively studied, motivated by their gained importance due to advancements in spintronics [2–6]. In contrast to half-metallic ferromagnets (HMFs) [7], only a few Heusler compounds (all of them with a rare earth metal at the Y position) have been successfully implemented as superconductors [8]. Pd_2YSn is the Heusler compound with the highest critical temperature (4.9 K) [9]. The coexistence of antiferromagnetism and superconductivity, demonstrating the manifoldness of the Heusler family, was reported for Pd_2YbSn [10] and Pd_2ErSn [11]. Many of the Heusler compounds have been reported to be HMFs [12,13], and several Co_2-based Heusler compounds have been used as electrodes in magnetic tunnel junctions [14,15]. The hexagonal compound Pd_2CeIn orders antiferromagnetically at 1.23 K [16]. D.B. de Mooij et al. [17] reported that Pt_2GdSn and Pt_2ErSn exhibit ferromagnetic (Tc=20 K) and paramagnetic behavior, respectively. Generally, Heusler compounds (X_2YZ) crystallize in the cubic $L2_1$ structure (space group $Fm\bar{3}m$), in which the lattice consists of interpenetrating fcc sublattices. The crystal structures of these compounds are shown in Fig. 1. Our paper is organized as follows. The theoretical background is presented in Section 2. The results and discussion are presented in Section 3. A summary of our results is given in Section 4.

2. Method of calculations

We have employed first-principles calculations [18,19] using the full-potential linearized augmented plane wave (FP-LAPW) method [20] as implemented in the WIEN2k code [21]. The exchange-correlation effects were described with the parameterization of the generalized gradient approximation (GGA) by Wu and Cohen (GGA-WC) [22], the local spin density approximation (LSDA) [23], GGA+U [24] and LSDA+U [25]. In the calculations reported here, we used the parameter $R_{mt}K_{max}$=9.5 to determine the matrix size (convergence), where K_{max} is the plane wave cut-off and R_{mt} is the smallest atomic sphere radius. We have chosen a muffin-tin (MT) radius of 2.6 a.u. for the Gd and Au atoms. For the In and Ag atoms, the MT radius is 2.5 a.u., and it is 2.4 a.u. for Cu atoms. Within these spheres, the charge density and potential are expanded in terms of the crystal harmonics up to an angular momenta of L=10. A plane wave expansion has been used in the interstitial region. G_{max} was set to 14, where G_{max} is defined as the magnitude of the largest vector in the charge density Fourier expansion. The Monkorst-Pack special k-points were performed using 1500 special k-points in the Brillouin zone for the Cu_2GdIn, Ag_2GdIn and Au_2GdIn compounds [26]. The convergence criteria for the total energy and force were set to 10^{-5} and 10^{-4} eV/Å, respectively. The GGA+U and LSDA+U calculations used an

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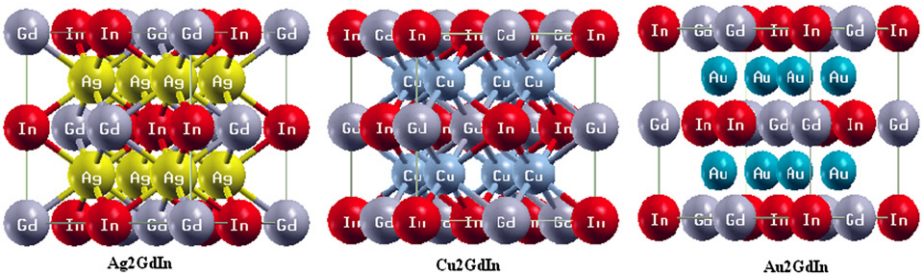

Fig. 1. The crystal structures of Cu_2GdIn, Ag_2GdIn and Au_2GdIn.

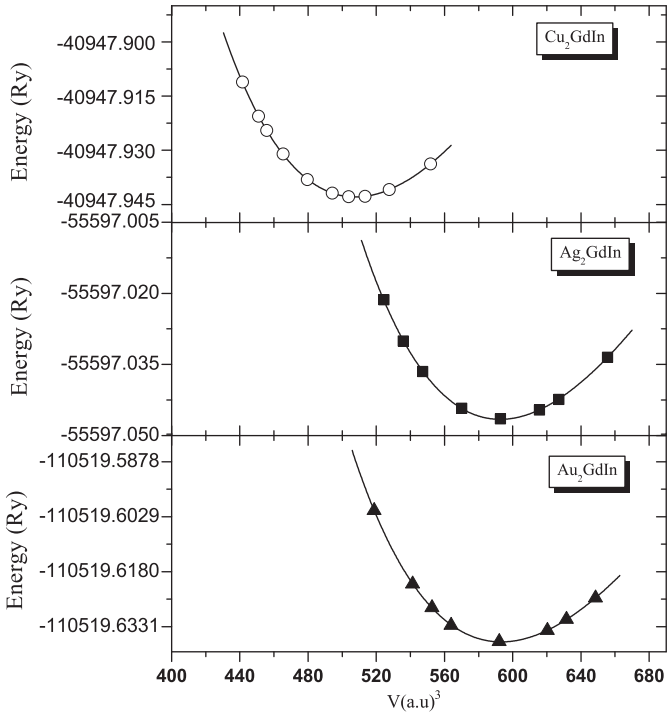

Fig. 2. The variations in the total energies as a function of the unit cell volumes of X2GdIn (X=Au, Ag or Cu).

Table 1
Lattice constant a (Å), bulk modulus B (in GPa), pressure derivative of bulk modulus B', elastic constants C_{ij} (in GPa), for Cu_2GdIn, Ag_2GdIn and Au_2GdIn compounds.

Compound		(GGA-WC)	GGA+U	LSDA	LSDA+U	Expt
Cu_2GdIn	a	6.70	6.587	6.50	6.498	6.447 [29] 6.641 [30] 6.6643 [31]
	B	82.60	95.234	109.32	106.209	–
	B'	4.47	5.029	5.52	4.692	–
Co_2CrBi [33]	B	132.7	–	–	–	–
	B'	5.20	–	–	–	–
Pd_2ZrAl [34]	B	151	–	–	–	–
Pd_2ZrIn [34]	B	141	–	–	–	–
Pd_2HfAl [34]	B	159	–	–	–	–
Pd_2HfIn [34]	B	150	–	–	–	–
	C_{11}	109.099	148.51	149.050	156.48	–
	C_{12}	70.011	85.42	86.944	84.20	–
	C_{44}	45.143	81.78	61.045	53.43	–
Ag_2GdIn	a	7.06	6.903	6.84	6.834	6.965 [28]
	B	81.27	86.435	96.66	97.088	–
	B'	5.52	5.513	5.16	5.407	–
	C_{11}	80.721	106.43	133.169	93.30	–
	C_{12}	65.816	98.35	81.903	103.51	–
	C_{44}	67.322	59.32	42.116	38.30	–
Au_2GdIn	a	7.06	6.938	6.86	6.857	6.94 [32]
	B	83.65	89.563	112.80	111.558	–
	B'	5.45	6.062	6.33	5.607	–
	C_{11}	89.301	125.39	119.770	107.32	–
	C_{12}	85.257	103.47	108.289	116.63	–
	C_{44}	57.101	51.70	50.572	45.91	–
Ni_2MnAl[37–40]	C_{44}	102[a], 64[b]	–	114.9[c],7.3[d]	–	–

[a] Ref. [37], PP/PAW_GGA-PW91.
[b] Ref. [38], FLAPW_GGA-PBE.
[c] Ref. [39], EMTO_LSDA.
[d] Ref. [40], FP-LMTO_LSDA.

Table 2
Shear modulus G, Young's modulus E (in GPa), Poisson's ration ν and Lamé's coefficients μ, λ and B/G (in GPa) for Cu_2GdIn, Ag_2GdIn and Au_2GdIn compounds.

Compound		(GGA-WC)	GGA+U	LSDA	LSDA+U
Cu_2GdIn	G	34.903	61.686	49.048	46.514
	E	91.782	152.197	128.001	121.766
	ν	0.315	0.234	0.305	0.309
	μ	34.903	61.686	49.048	46.514
	λ	8.139	15.355	11.672	10.982
	A	28.239	2.592	8.809	1.478
	B/G	2.366	1.883	2.228	2.283
Ag_2GdIn	G	43.374	37.208	35.523	20.938
	E	110.469	97.617	94.938	58.601
	ν	0.273	0.312	0.336	0.399
	μ	43.374	37.208	35.523	20.938
	λ	10.748	8.734	7.822	3.365
	A	9.033	14.683	1.643	–
	B/G	1.873	2.323	2.721	4.637
Au_2GdIn	G	33.069	35.404	32.639	25.684
	E	87.657	93.846	89.305	71.560
	ν	0.325	0.324	0.368	0.393
	μ	33.069	35.404	32.639	25.684
	λ	7.516	8.047	6.341	4.317
	A	2.309	4.717	1.965	4.343
	B/G	2.529	2.529	3.456	–
Ni_2MnAl [37–40]	G	32[a], 10[b]	–	15.6[c], 18.8[d]	–

[a] Ref. [37], PP/PAW_GGA-PW91.
[b] Ref. [38], FLAPW_GGA-PBE.
[c] Ref. [39], EMTO_LSDA.
[d] Ref. [40], FP-LMTO_LSDA.

effective parameter $U_{eff}=U-J$, where U is the Hubbard parameter and J is the exchange parameter. We set $U=7.07$ eV and $J=0.0$ eV. These parameters were sufficient to give good structural and elastic moduli.