Structural, Chemical Bonding, Electronic and Magnetic Properties of XY₃

(X = Al, Ga and Y = V, Nb, Cr, Mo) Compounds

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(Received August 18, 2013)

The metallic behavior of the band gap of intermetallic compounds has large applications in superconductivity, nickel-metal hydrides batteries, semiconductors, and heating materials. The presence of transition elements makes them more attractive for magnetic applications. In this work we studied the structural, electronic, chemical bonding, and magnetic properties of binary intermetallic compounds XY_3 (X = Al, Ga and Y = V, Nb, Cr, Mo). These compounds were investigated by using full potential linearized augmented plane wave plus local orbitals method. The exchange correlation potential of generalized gradient is used. Our calculated lattice constants are in good agreement with experimental values. The band structures of these compounds are purely overlapping across the Fermi level. The bonding is mainly covalent in these compounds. The density of states of the compounds shows that the major contribution arises from *d*-states of anions. The investigation carried out shows that the most of these compounds have ferromagnetic nature, while few are diamagnetic. On the basis of this study it is expected that these compounds can be used as a best moulds for future study on similar compounds.

DOI: 10.12693/APhysPolA.127.770

PACS: 71.15.Ap, 71.20.-b

1. Introduction

Materials like intermetallics and there alloys have been an active field of study for last 20 years [1]. It is because they are indispensable in many applications and have additional breakthrough especially for high storage structural materials, magnetic materials, hydrogen storage materials [2], semiconductors, superconductors, refractory alloys, high strength materials, dental amalgams (AgSn₃), antifriction materials, metallic glasses, contact layers or barrier layers for microelectronics (TiSi₂), coating tools and dies, furnace hardware, cladding, heating materials, aerospace, piping of chemical industries [3].

Intermetallic compounds contain two or more metallic elements with one or more optionally non-metallic, bounded by dominant intermetallic bond, with different phase structure from that of constituents [4]. They are divided on the basis of number of constituent atoms into alkali metals binary intermetallics, noble binary intermetallics, group 13 binary intermetallics, ternary intermetallics etc. [5]. Generally binary intermetallics are represented by symbol $A_x B_x$, where A represent stable hydride forming elements whilst B is for unstable one. Binary intermetallics have been divided on the basis of their structural differences into five categories i.e. AB, AB_2 , AB_3 , AB_5 , A_2B_7 , and magnesium based alloys [6]. Where AB includes AlGa [7], FeAl, NiAl, TiAl, they are of low cost and are easily used for microfibrication, corrosion and oxidation resistance, fire resistance, aircraft industry and carburization [8]. AB₂ compounds include AuI₃ [9], MgCu₂, MgZn₂, and Laves phases. These compounds are important from commercial point of view because they are used in nickel-metal hydrides batteries [6, 10], some of them are very good electrical conductors [9]. Ce_2Ni_7 type and $CaCu_5$ type compounds are examples of A₂B₇ and AB₅, respectively. Like AB₂, AB₅ are also important and used in nickel-metal hydrides batteries. However since they have low hydrogen storage capacity so therefore they have limited applications [6, 10– 13]. AB₃ intermetallics, in which A is a p-block element of group III in periodic table, i.e. Al, Ga while B includes d-block elements also termed as transition elements of periodic table i.e. V, Nb, Cr, and Mo. The studied literatures clear that these intermetallics have large applications in magnetic and superconductivity but their structural, electronic and magnetic properties have not been explained.

2. Methodology

In this work we calculate the properties of these compounds by using the full potential linearized augmented plane wave (FP-LAPW) [14, 15] method implemented

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in the WIEN2K package [16]. The computational investigation of the ground state properties of the materials [17] was first performed by structural optimization of the materials, and the generalized gradient approximation (GGA) parametrized by Wu and Cohen [18] was used to account for the exchange correlation effects. The basis set is determined by considering two regions inside the unit cell; one is non overlapping spheres and the other one is interstitial region. Inside the first region a linear combination of radial function times the spherical harmonics is used. In the second region a plane wave expansion is augmented by atomic sphere. In order to achieve the energy convergence of the eigenvalue, a cut off $K_{\text{max}}R_{\text{MT}} = 7.0$ for the expanded wave function of the plane waves in the interstitial region was chosen as shown in Tables I and II, where $R_{\rm MT}$ implies the minimum radius of the sphere and K_{\max} provides the magnitude of the K-vector. Also, the charge density is Fourier expanded up to $G_{\text{max}} = 12$ and the maximum value of l inside the sphere is $l_{\text{max}} = 10$. We have used $1000 \ k$ -points with the tetrahedral method for the Brillouin zone integration.

	TABLE I
$R_{\rm MT}$, K-points, $R_{\rm MT}K_{\rm max}$ values of	Intermetallic
compounds for configuration $(0, 0.5,$	0).

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Compounds		$R_{\rm MT}$	K-points	$R_{\rm MT}K_{\rm max}$
AlV ₃	Al	1.99	1000	7.00
	V	1.85		
$AlNb_3$	Al	2.00	1000	7.00
	Nb	1.80		
AlMo ₃	Al	2.00	1000	7.00
	Cr	1.80		
${\rm GaV}_3$	Ga	1.99	1000	7.00
	V	1.90		
GaNb_3	Ga	2.03	1000	7.00
	Nb	2.00		
${ m GaCr}_3$	Ga	1.99	1000	7.00
	Cr	1.90		
${ m GaMo_3}$	Ga	1.96	1000	7.00
	Mo	1.90		

3. Results and discussion

3.1. Structural properties

The intermetallic compounds AB_3 (A = Al, Ga, and B = Cr, Mo, V, Nb) have space group No. 221 (Pm-3m) with two atoms per unit cell. The unit cell structure of these compounds with configuration I (0, 0.5, 0) and II (0, 0.5, 0.5) is depicted in Fig. 1. In configuration I, the A cation is at the corners of the cube while the B anion is at the middle of the axis of the unit cell. In configuration II, A cation is at the corners of the unit cell while the B anion is at the center of the faces of the unit cell.

The structural properties of the said intermetallic compounds are predicted by optimizing the volume, i.e. minimizing the total energy of the unit cell with respect 771

$R_{\rm MT},$	K-poi	nts	and	$R_{\rm MT}K_{\rm max}$	values	\mathbf{of}	Inter-
metall	ic com	poui	ds f	or configura	tion (0	, 0.5	, 0.5).

Compounds		$R_{\rm MT}$	K-points	$R_{\rm MT}K_{\rm max}$
AlV_3	Al	2.00	1000	7.00
	V	1.90		
AlNb ₃	Al	2.00	1000	7.00
	Nb	1.90		
$\mathrm{AlM}\mathrm{o}_3$	Al	2.00	1000	7.00
	Cr	1.90		
${\rm GaV}_3$	Ga	2.00	1000	7.00
	V	1.80		
GaNb_3	Ga	2.00	1000	7.00
	Nb	1.90		
${ m GaCr}_3$	Ga	2.20	1000	7.00
	Cr	2.00		
$GaMo_3$	Ga	2.00	1000	7.00
	Mo	1.90		



Fig. 1. Structures of AB_3 intermetallic compounds for configuration I and II.

to the variation in the unit cell volume. The unit cell energy versus volume plot for only $GaNb_3$ is shown in Fig. 2 as a prototype. The minimum position of the equation of state (EOS) defines the equilibrium state of the system. The minimum energy is known as the ground state energy while the volume corresponding to this energy is known as ground state volume. Lattice parameters are evaluated using this unit cell volume at zero pressure. The structural parameters like lattice constant,



Fig. 2. EOS of AB_3 intermetallic compounds for configuration I (upper) and Configuration II (lower).

bulk modulus, the pressure derivative of bulk modulus and the unit cell volume as well as energy are given in Table III and Table IV for configuration I and II, respectively. Lattice constants of these compounds in configuration II are smaller than those in configuration I. The lattice parameters for the configuration I are in good agreement with experimental and other theoretical predictions. However, for configuration II, there are no previous theoretical or experimental works to compare. Thus, the unit cell volume, bulk modulus and energy per unit volume for this configuration can be considered as reference data for future experimental and theoretical works.

TABLE III

Unit cell volume V₀ [Å³], lattice parameters a [Å], bulk modulus B [GPa], pressure derivative of bulk modulus B', ground state energy E_0 [Ry] of AB₃ intermetallics for configuration I.

Com	pounds	V_0	a [Å]	B [GPa]	B'	E_0 [Ry]
AlV_3	this cal.	767.80	4.84	31.58	0.73	-6178.33
	other cal.	-	4.81^{*}	-	_	-
	expt.	-	4.80^{*}	-	-	-
$AlNb_3$	this cal.	717.91	4.74	79.87	5.49	-23403.81
	other cal.	-	5.19^{*}	-	-	-
	expt.	-	5.13^{*}	-	-	-
AlMo ₃	this cal.	638.26	4.56	100.38	4.65	-24778.25
	other cal.	_	4.95^{*}	_	-	-
	expt.	_	4.95^{*}	_	-	-
GaV_3	this cal.	748.50	4.80	38.65	1.49	-9580.48
	other cal.	_	4.82^{*}	_	-	-
	expt.	-	4.79^{*}	_	-	-
GaNb_3	this cal.	734.55	4.77	88.82	4.34	-26805.92
	other cal.	-	5.18^{*}	_	-	_
	expt.	-	5.12^{*}	-	-	-
${\rm GaCr}_3$	this cal.	765.22	4.84	40.79	4.22	-10183.70
	other cal.	-	4.65^{*}	-	-	-
	expt.	-	4.68^{*}	-	-	-
${\rm GaMo_3}$	this cal.	809.99	4.93	251.56	5.00	-28180.23
	other cal.	_	4.94^{*}	-	-	-
	expt.	-	4.93^{*}	-	-	-
* — Re	f [19]					

The bulk modulus for material can be defined as the change in pressure to the fractional volume of compression which can be written as

$$B = -V\frac{\partial P}{\partial V}.\tag{3.1}$$

Since the hardness depends on the bulk modulus, which is a function of both strength of intermetallic bonding and the rigidity of the frame work of lattice [19]. The calculated bulk modulus values listed in Tables III and IV clearly show that the compounds in configuration II have high bulk moduli as compared to configuration I. Hence the compounds are much harder when anion B is at the faces of the cube than at middle of the axis.

Unit cell volume V₀ [Å³], lattice parameters a [Å], bulk modulus B [GPa], pressure derivative of bulk modulus B', ground state energy E_0 [Ry] of AB₃ intermetallics for configuration II.

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Com	pounds	V	[a [Å]	B [GPa]	B'	E_0 [Ry]
AlV ₃	this cal.	362.02	3.77	181.63	3.49	-6179.03
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
AlNb ₃	this cal.	461.35	4.09	160.89	4.46	-23404.52
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
AlMo_3	this cal.	407.82	3.92	224.54	3.71	-24779.52
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
GaV_3	this cal.	355.10	3.75	176.67	4.36	-9581.12
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
GaNb_3	this cal.	452.77	4.06	169.61	4.04	-26806.61
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
GaCr_3	this cal.	319.18	3.62	236.91	4.47	-10190.41
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	-
${\rm GaMo}_3$	this cal.	402.04	3.91	230.71	4.69	-28181.15
	other cal.	-	-	-	-	-
	expt.	-	-	-	-	_

3.2. Band structure of AB_3 intermetallic

The electronic band structure of the herein studied AB_3 intermetallic compounds are computed at the optimized lattice parameters within the GGA approximation for both configurations and with spin up and spin down electronic orientation. Figure 3 shows the computed



Fig. 3. Electronic structures of AlV_3 intermetallic compound for position I and II with spin up and spin down electronic orientation.

energy band structure along the high symmetry directions in the Brillouin for only AlV_3 as a prototype. In view on this figure, it seen that the band structures (BS) of these compounds at the Fermi energy (E_F) level are thickly populated by overlapping valence band (VB) and conduction band (CB) states, revealing that they have a metallic nature (no energy band gap).

3.3. Density of states

To further explain the nature of the electronic band structure, we have also calculated the total and partial densities of states (TDOS and PDOS). They are displayed in Figs. 4–10.

The calculated TDOS and PDOS of AlV₃ in Fig. 4 show that the electronic bands have overlapping nature across the Fermi level. The maximum contribution to the TDOS in spin up mode is from the V 3d states. The contribution from Al 3s appears at energy of -5 eV. In spin down orientation, V 3d and Al 3s states remain the same whilst V 3d states shift into the conduction band. Splitting of V 3d states in spin up mode reveal that V ($d_{xz} + d_{yz}$), V (d_{xy}) and V (d_{z2}) show maximum contribution to V 3d states in valence band and conduction band. The spin down mode presents that these states shift into the conduction band. Configuration II of AlV₃ shows that the Al 3p state has its maximum contribution to TDOS in both spin channels. The contribution from Al 3s state appears at energy of -7.5 eV in both channels. From the band structure and PDOS, one can see that there exists hybridization between the Al 3s, V 3d and Al 3p states at around 7.8 eV. Splitting of V 3d state shows a major contribution of V $(d_{xz}+d_{yz})$ at the Fermi level.

Figure 5 shows that the maximum contribution to TDOS of $AlNb_3$ is from Nb 4d in both modes with majority in the conduction band. In spin up mode, the contribution of Al 3s appears at -4 eV, whilst Al 3d contribution arises above and below the Fermi level. In spin down mode, contribution of PDOS remains the same. Splitting of AlNb₃ reveals that in spin up mode, major contribution to Nb 4d arise from the Nb $(d_{xz}+d_{yz})$ at the Fermi level. The degenerated Nb d_{z2} and Nb d_{xy} states share their contributions in the conduction band. In spin down mode, the contribution remains the same with no prominent difference. In configuration II, the Al 3d states hybridize with the Nb 4d states at energy -2.5 eV which overlap into the conduction band in descending nature. The Al 3s contribution appears at energy -4.0 eV with increase of number of DOS/eV to both modes of orientation.

The hybrid contribution of Al 3s with Al 3d and Nb 4d arises at -4.0 eV and 5.8 eV in both modes. Splitting of PDOS shows that Nb $(d_{xz} + d_{yz})$ have a maximum contribution to Nb 4d. Its share arises at the Fermi level and conduction band in both modes of electronic orientation.



Fig. 4. DOS and PDOS of AB₃ intermetallic compounds for configuration I (0, 0.5, 0) and II (0, 0.5, 0.5) with spin up and spin down states, the top of the valence band is marked as E_F at 0 eV.



Fig. 5. As Fig. 4, for $AlNb_3$ (top) and $AlMo_3$ (bottom).



Fig. 6. As Fig. 4, for GaV_3 (top) and $GaNb_3$ (bottom).



Fig. 7. As Fig. 4, for $GaCr_3$ (top) and $GaMo_3$ (bottom).

In AlMo₃ the prominent contribution to TDOS is from Al 3s, Al 3p, and Mo 4d in both modes as shown in Fig. 6. The major contribution of Mo 4d appears at the Fermi level in both electronic orientations. Contribution of Al 3s first appear at -5.0 eV and then at -2.8 eV and $7.5~\mathrm{eV}$ with maximum in spin down mode. The hybrid nature of Al 3s with Al 3p and Mo 4d is clear in Fig. 6. Splitting of PDOS reveals that the maximum contribution to Mo 4p arise from p_z and $p_x + p_y$ states. Splitting $d_{xz} + d_{yz}$ share prominently to Mo 4d in both modes of orientations. In configuration II, the contribution of AlMo₃ to TDOS is from Al 3s, Al 3p and Mo 4d. Contribution of these PDOS is the same in both electronic orientations. Splitting of PDOS shows that maximum contribution to Mo 4p is from p_z and $p_x + p_y$ in both mode of orientation.

Figure 7 shows that the maximum contribution of GaV_3 to TDOS is from V 3d in both modes of orientation. In spin up mode, the V 3d appears at -2.5 eV and expands into conduction band. In spin down mode it appears above the Fermi level. The share of Ga 4s in spin up orientation appear at -6.0 eV. In spin down mode it shifts toward the Fermi level with a small energy gap of 0.02 eV. Splitting of PDOS shows that the maximum contribution to V 3d is from V $(d_{xz} + d_{yz})$ above and below the Fermi level. Contribution of V (d_{xy}) is prominent with a peak value just above the Fermi level. The major contribution of V (d_{z2}) appears at 0.02 eV. Split states V (d_{x2y2}) appear in the valence band with decreasing nature across the Fermi level into the conduction band. In spin down mode, the splitting of states remains the same but shift into the conduction band. In configuration II the maximum contribution to TDOS is from V 3din both modes. It appears at -4.5 eV and expands across the Fermi level into conduction band. The Ga 4s states appear at -5.4 eV in spin up and shift towards the Fermi level in spin down mode of orientation as shown in Fig. 7. Splitting of PDOS reveals that the maximum contribution to V 3d in both valence and conduction bands is from V $(d_{xz} + d_{yz})$ in both modes.

Configuration I of GaNb₃ displayed in Fig. 8 shows that the Ga 4s and Nb 4d contribute dominantly to TDOS in both spin channels. Splitting of GaNb₃ shows that the maximum contribution to Nb 4d arises from Nb (d_{xy}) above the Fermi level in both up and down modes. The contribution due to other split states expands up to energy of 14.5 eV. In configuration II, the contribution to TDOS is similar in nature to AlNb₃ in both mode of orientation. However, splitting results reveal that the maximum contribution to Nb 4d is from Nb (d_{xy}) in both mode of orientation. It appears at energy -6.7 eV and expands into conduction band with maximum value at 2.8 eV.

Figure 9 shows that the major contribution of $GaCr_3$ to TDOS in spin up mode is from Cr 3d which appears at -2.8 eV and Ga 4s appears at -5.8 eV. In spin down mode the Cr 3d state appear completely above the Fermi level whilst Ga 4s appears at same point with a little shift towards Fermi level. Splitting of PDOS shows that

the maximum contribution to Cr 3d is from Cr $(d_{xz} + d_{yz})$ in spin up mode. In spin down mode the splitting shifts into the conduction band. In configuration II, the dominant contribution to TDOS is from Cr 3d in both mode of orientation. The Ga 4s contribution appears at -7.0 eV and hybridizes with Cr 3d at -4.5 eV and 4.0 eV. The splitting of GaCr₃ shows that the maximum contribution to Cr 3d is from Cr $(d_{xz} + d_{yz})$ at the Fermi level and conduction band in both electronic orientations.

Figure 10 shows that Ga 4s and Mo 4d contribute prominently to TDOS of GaMo₃ in both modes of orientation. The contribution of Mo 4d appears at -4.0 eV in spin up mode whilst contribution of Ga 4s appears at -5.8 eV. In spin down mode the contribution of PDOS is almost the same with a shift of Mo 4d into the conduction band. In configuration II, the hybridization of Ga 4s with Mo 4d appears at -4.0 eV and 5.0 eV in both up and down modes. The splitting results show that the contribution to Mo 4d is from Mo (d_{x2y2}) in both modes.

3.4. Electron density

The electron density of $AlMo_3$ for configurations I and II is shown in Fig. 5 as a prototype. The bonding nature of these compounds is covalent with thick electron density around transition elements. In configuration I, the electron density is larger in spin up channel than that in spin down. It is further noted that the distributions of the electrons is overlapping largely in spin up state as compared to spin down state in this configuration. Therefore, the covalent bonding is much stronger in spin up channel as compared to spin down. The results of configuration II show that the electrons population in spin up channel is larger than that in spin down channel. AlNb₃ and GaMo₃ show a covalent bonding while the remaining compounds show an ionic nature.

3.5. Magnetic properties

To calculate magnetic properties of AB₃ intermetallic compounds we perform spin polarized calculations. The magnetic moments of these compounds for configurations I and II are shown in Tables V and VI. Table V shows that AlV₃, GaV₃, GaCr₃, GaMo₃ have ferromagnetic behavior, whilst AlNb₃, AlMo₃ and GaNb₃ compounds have diamagnetic nature. The major contribution to the total magnetic moment of these compounds arises from S2 transition elements, i.e. V, Nb, Cr, Mo. The values of magnetic moments for transition elements decrease in going from V to Nb and Cr to Mo. In AlMo₃ both the spheres have negative values, which support one another into diamagnetic behavior. In GaV_3 the S1(Ga) have negative value which show antiparallel response to S2(V). Since V has major contribution so the resultant value is ferromagnetic. In GaCr₃ the behavior of S1(Ga) atom remains the same. Table VI shows that in configuration II (0.5, 0.5, 0), the overall behavior of these compounds is diamagnetic. However, GaMo₃ shows small ferromagnetic behavior.



Fig. 11. Electron density of $AlMo_3$ intermetallic compounds for configuration I (0, 0.5, 0) and II (0, 0.5, 0.5) with spin up and spin down electronic orientations.

4. Conclusion

The properties of AB_3 (A = Al, Ga and B = V, Nb, Cr, Mo) intermetallic compounds studied in this work are calculated by using the GGA technique which lead to the following conclusions:

- The lattice constant obtained from the calculation are in good agreement with the experimental and other theoretical values.
- The calculated bulk modulus values of these compounds show that the compounds have more strength in configuration II.
- Results obtained for band structures have overlapping mode across the Fermi level which show their metallic nature.
- The study of electronic structure allows us to point out the bonding nature of these compounds, which is covalent for all the compounds of both configurations. However in configuration II, $AlNb_3$ and $GaMo_3$ have ionic behavior.

- The DOS calculation shows that the major contribution of different states near the Fermi level is from *d*-states.
- The DOS shows that AlV₃, GaV₃, GaCr₃ and GaMo₃ compounds have ferromagnetic behavior whilst the rest of compounds have diamagnetic trend in configuration I. In configuration II most of the compounds have diamagnetic nature while GaMo₃ shows small ferromagnetic behavior.

TABLE V

Calculated spin magnetic moments of mixed charge density for configuration I (0.5, 0, 0) of AB₃ intermetallic with magnetic moment. m^{inst} (interstitial), m^{s1} (sphere 1), m^{s2} (sphere 2), m^{c} (cell).

Compounds	$m^{ m inst}$	m^{s1}	m^{s2}	$m^{ m c}$
AlV ₃	3.53379	0.00292	2.09644	9.82603
$AlNb_3$	0.23616	0.00353	0.04553	0.37626
$AlMo_3$	-0.22354	-0.00683	-0.08088	-0.47301
${ m GaV_3}$	3.07540	-0.00854	2.25146	9.82122
GaNb_3	0.21905	0.00371	0.06323	0.41244
$GaCr_3$	3.13117	-0.07100	3.31824	13.01489
${ m GaMo_3}$	3.80325	0.00508	1.61200	8.64433

TABLE VI

Calculated spin magnetic moments of mixed charge density for configuration II (0.5, 0.5, 0) of AB₃ intermetallic with magnetic moment m^{inst} (interstitial), m^{s1} (sphere 1), m^{s2} (sphere 2), m^{c} (cell).

Compounds	m^{inst}	m^{s1}	m^{s2}	m^{c}
AlV ₃	0.08555	-0.00044	0.07651	0.31465
$AlNb_3$	-0.00099	-0.00008	0.00009	-0.00079
$AlMo_3$	-0.00154	0.00013	0.00005	-0.00127
${ m GaV_3}$	0.09324	-0.00064	0.06896	0.29947
GaNb_3	-0.00217	0.00014	-0.00051	-0.00355
$GaCr_3$	0.00932	-0.00023	0.03344	0.10942
${ m GaMo}_3$	0.51432	0.00198	0.65937	1.17567

Acknowledgments

Authors (Khenata and Bin Omran) acknowledge the financial support by the Deanship of Scientific Research at King Saud University for funding the work through the research group project No. RPG-VPP-088.

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