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First Principles Study on Structural and Electronic Properties of REAg (RE= Y, La, Pr and Er) Intermetallics

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Abstract
We The structural, electronic and mechanical properties of binary B_2 – type CsCl structured intermetallic compounds of Ag (ReAg, Re= Y, La, Pr and Er) have been studies systematically by means of first principles density functional theory within generalized gradient approximation. Ground state properties such as lattice constant (a_0), bulk modulus (B) and its pressure derivative (B′) are obtained. The present results are in good agreement with the experimental and other theoretical calculation available. Amongst all the Intermetallics is found ErAg to be most ductile due to the presence of strong metallic bonding.
Keywords: Intermetallic compounds; Density Functional Theory; Ductility; Electronic Structure.

1. Introduction

Intermetallic compounds are formed when two or more metals are mixed together in certain proportions and react to produce a solid phase that is distinctively different from the constituent elements. Much of the changes in character are found due to a difference in the chemical bonding that bind the atoms of the phase together. This can profoundly alter the character of the new phase in terms of crystal structure, chemical, mechanical and electrical properties. Due to long-range ordering and specific properties, the intermetallic alloys are assumed to fill an existing gap between structural ceramics and classical metallic alloys. The intermetallics exhibit interesting mechanical and thermal properties such as high tensile strength, good ductility, high corrosion resistance and thermal stability [1-7]. In intermetallic compounds the absence of'*d*' like electrons near the Fermi level accounts for the observed ductility in 90% of the compounds [6]. In the present study only binary alloys, with particular attention to the formation of intermediate phases, which crystallize is in CsCl –type structure (B_2 phase) are considered.

In pure silver, the atoms are bound together with metallic bonds. The noble metal Ag is characterized by their positive reduction potentials against the hydrogen, high densities, high melting temperatures, high electrical and thermal conductivity, optical reflectivity and catalytic properties [8]. However, silver is ductile but it is soft. The electronic density of states (DOS) near Fermi surface is nearly the same of all noble metals. The small energy differences in DOS between their outer *s* and *d* electronic states result in multiple oxidation states [8]. An alloying behaviour of silver with its intermetallic chemistry has its own particular characteristics, which are important both as a sound basis for further study and for a great variety of applications (electronics fabrication, electrical engineering, coins and medals, jewellery, without lead soldering, high danced surgical instruments, pen nibs, dental materials, coatings, etc.)[10].

The CsCl –type binary intermetallic compounds of silver with rare-earth metals were studied by Chao *et. al.* [9] performed using x-ray diffraction technique. The general alloying behaviour and stability of silver is summarized on the basis of literature data and experimental result, by Ferro *et. al.* [10]. The structural stability of many binary intermetallic compounds was estimated by Curtarolo *et. al.* [11] by using *ab-initio* LDA/GGA computation. Baranov [12] predicted structural stability of pure elements and binary intermetallic compounds assuming the density of atoms as stationary and un-deformable in internal and external spherical symmetrical shell. Nakamura [13] has determined the elastic moduli from the velocity of an ultrasonic wave in a single crystal of materials.

From recent study, it has been possible to predict ductility or brittleness from the electronic nature of AB type intermetallics, either by using semi-empirical theory or first-principles calculations [6].

Although there is a lot of work on the structural stability and mechanical properties of these compounds are available in the literature [8, 10, 11], but very less attention has been paid for electronic properties. Lack of the study of these properties has motivated us for a systematic study of these compounds. In the present chapter, we primarily aim to understand the electronic and mechanical properties of this group of intermetallic viz YAg, LaAg, PrAg, and ErAg, using *ab-initio* full potential-linearized augmented plane wave (FP-LAPW) method. We report the ground state properties and electronic band structures. We also critically examine their ductile property, by calculating the Density of states.

2. Methodology

The present calculations have been performed by using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k package [16], based on the density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzrhof (PBE) is used for the exchange and correlation effects [17]. In order to achieve convergence, we expand the basis function up to $R_{MT}*K_{max}= 7$ where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest $\boldsymbol{k}$ vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is $l_{max}= 10$ while the charge density is Fourier expanded up to $G_{max}= 12$. The self-consistent calculations are considered to converge when the total energy of the system is stable within 10^{-4} Ry. A dense mash of 1000 $\boldsymbol{k}$ points and the tetrahedral method [18] have been employed for the Brillouin zone integration. The total energies are fitted to Birch [19-20] equation of state to obtain the ground state properties.

3. Result and Discussion

3.1 Structural Properties

Firstly, the non-spin polarized electronic band structure calculations are carried out to obtain the total energy of the REAg (RE= Y, La, Pr and Er) intermetallic compounds using the first principles FP-LAPW method.

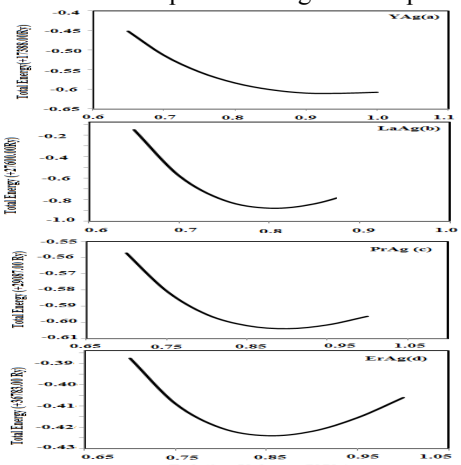

Figure 1(a) – (d): Variation of total energy of YAg(a) , LaAg(b), PrAg(c) and ErAg(d) with relative volume in CsCl- Structure.

In order to calculate the ground state properties of these intermetallics, the total energies are calculated in B_2 phase for different volumes around the equilibrium cell volume V_0. The calculated total energy versus reduced volume plots for these compounds are given in Fig.1. A inspection of Fig 1, reveals that all the compounds are stable in B_2 – phase with lowest energy at ambient condition and well agree with other result [11, 12].

The calculated total energies are fitted to the Birch equation of state [17] to determine the ground state properties like lattice constants a_0, bulk modulus B and its pressure derivative B'. The ground state properties of these compounds are presented in Table 1.

Table 1: Calculated equilibrium lattice parameter a_0 (Å), bulk modulus B_0 (GPa) and pressure derivative B_0' of YAg, LaAg, PrAg and ErAg in CsCl structure.

Solids		a_0 (Å)	B_0 (GPa)	B_0'	$N_{(EF)}$ (eV)	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
YAg	Present	3.536	90.60	4.673	0.689	85.05	53.26	48.24
	Experimental	3.619[a]	-	-	-	84.00[a]	56.00[a]	48.00[a]
LaAg	Present	3.730	60.66	4.618	1.518	105.71	68.71	53.54
	Experimental	3.812[a]	-	-	-	-	-	-
PrAg	Present	3.596	59.94	4.7	0.528	128.71	84.98	84.92
	Experimental	3.718[a]	-	-	-	-	-	-
ErAg	Present	3.394	96..35	4.941	0.560	85.66	76.37	57.46
	Experimental	3.577[a]	-	-	-	-	-	-

[a]Ref [6]

The ErAg bulk modulus value is highest, showing that it is most compressible as compared to other REAg intermetallic compounds. The calculated values of lattice parameters are in good agreement with the

experimental values [6]. The small variations in our calculated parameters with the other results due to the methodology FP-LAPW in which the full potential for all the electrons is considered.

3.2 Electronic Properties

To understand exact electronic properties of REAg intermetallics we have calculated the qualitative picture of their electronic band structure (BS) and Density of states (DOS). The calculated electronic band structure along the principal symmetry directions and total density of states of REAg compounds in B_2 – phase which are presented in Fig. 2 where Fermi level is considered at origin.

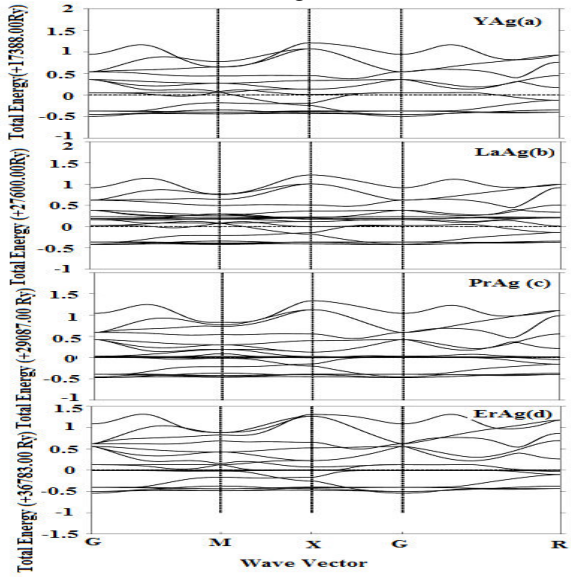

Figure 2(a)-(d). Band structure for YAg(a), LaAg(b), PrAg (c) and ErAg(d) in CsCl structure.

The total and partial densities of states (DOS) for these compounds at ambient pressure are presented in Fig 3 and Fig 4

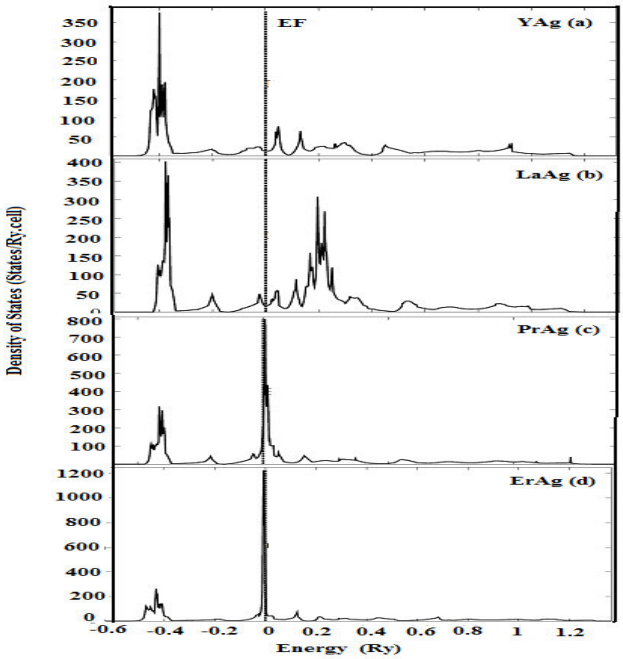

Figure 3(a)-(d): Total Density of states for YAg(a), LaAg(b), PrAg (c) and ErAg(d) in CsCl Structure .

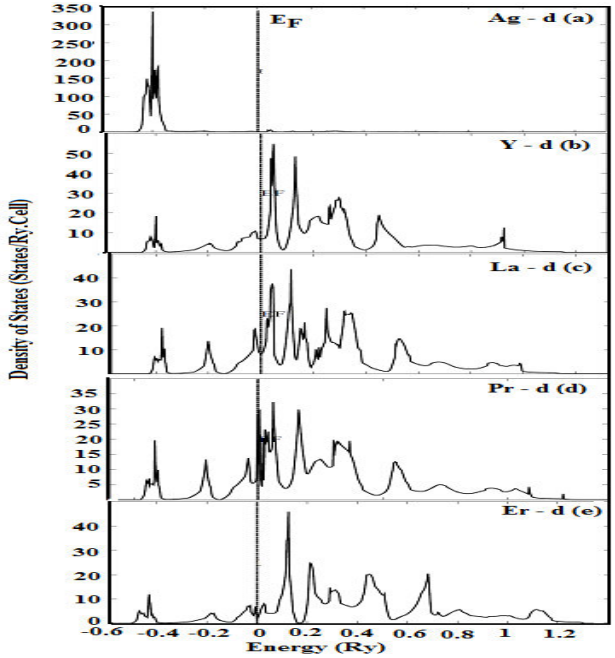

Figure 4(a)-(e): Partial Density of states of d- orbital for Ag(a), Y(b), La (c), Pr(d) and Er(e) in CsCl Structure .

From Fig 2 it is revealed that the REAg compounds are metallic in nature and the region around the Fermi energy is densely populated by hybridization of RE-*d,f* and Ag-*s,p* bands. It is revealed from Fig 2 and Fig 3 except for ErAg, in all the REAg compounds the lowest lying band is due to RE '*p*', '*d*' '*f*' , Ag '*p*' and Ag '*s*' states. In ErAg however the metalicity is observed due to crossing of Er '*p*' '*f*' and Ag '*p*' states at Fermi level.
To understand learn about ductile/brittle behaviour of REAg intermetallic compounds [6] in Fig 5.4.we have compared the position of Ag-*d* and RE-*d* bands at the Fermi level with the help of partial dos of *d* orbital for Y, La, Pr, Er and Ag
From Fig 4.it can be observed that ductile behaviour appears to be determined by the transition metal element (Ag) in the compound and is relatively insensitive to the identity of rare earth element. The trends can be explained on the basis of electronic configurations of the B_2 type REAg compounds. From above diagram it is also observed that ErAg and YAg are more ductile compounds rather than LaAg and PrAg due to the delocalized'*d*' states of Ag and RE atom.

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