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Ab-initio Calculations of Structural, Electronic, Elastic and Mechanical Properties of $REIn_3$ and $RETl_3$ (RE= Yb & Lu) Intermetallic Compounds

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Abstract

A theoretical study of structural, electronic and elastic properties of $REIn_3$ and $RETl_3$ (RE = Yb & Lu) intermetallics have been investigated systematically using first principles density functional theory. The calculations are carried out using generalized gradient approximation (PBE-GGA) for the exchange correlation potential. The ground state properties such as lattice parameter (a_0), bulk modulus (B) and its pressure derivative (B′) are calculated which show well agreement with the experimental and other available theoretical results. We first time predict elastic constants for these compounds. From energy dispersion curves, it is found that these compounds are metallic in nature. Both of these compounds are found to be ductile in nature in accordance with Pugh's criteria..

Keywords: Rare-earth; Density functional theory; Elastic constants.

1. Introduction

Rare earth intermetallics are in a prominent situation not only from a fundamental point of view but also for the large number of technological applications, in particular in the field of permanent magnets. They play an important role in a large range of current research fields, in particular those devoted to heavy fermions, valence fluctuations, Kondo lattices, magnetostrictive materials, permanent-magnet materials, spin glasses and random anisotropy systems [1]. Rare-earths (RE) based intermetallics REX_3 (X= In, Tl), which crystallizes in $AuCu_3$ type structure, are of considerable technological and scientific interest due to extraordinary magnetic properties and industrial applications. Ambiguous magnetic behavior of some Yb-compounds has been studied by Klasse *et.al.* [1]. Complicated metamagnetism of many antiferromagnet and divalency in $YbIn_3$ have been studied by Guegan *et.al.* [2]. Valency of rare earths in RIn_3 and RSn_3 and *ab-initio* analysis of electric field gradients have been investigated by Asadabadi *et.al.*[3]. Very few experimental as well as theoretical studies are reported on REX_3 compounds, which lighted us to perform the present study. The effect of pressure on the magnetic susceptibility of rare earth intermetallic compounds GdM (M =Cu, Ag, Mg) and RIn_3 (R = Gd, Tb, Dy) has been investigated by Grechnev [4]. The effect of spin polarization on the structural properties and the electric field gradient (EFG) on Sn, In, and Cd impurities in RSn_3 (R = Sm, Eu, Gd) and RIn_3 (R = Tm, Yb, Lu) compounds have been studied by Asadabadi *et.al.* [5] using the scalar-relativistic full potential linearized augmented plane wave method. They reported that GGA + Spin Polarization is successful in predicting the larger lattice parameter and the dramatic drop of Electric Field Gradient (EFG) for (R = Eu, Yb) relative to other rare-earth compounds. The magnetic properties and the lattice parameters for 13 compounds of the composition RIn_3 (Cu_3Au structure) are reported by Buschow et.al. [6].

The rare earth intermetallics $REIn_3$ and $RETl_3$ (RE = Yb, Lu) crystallizes in cubic $AuCu_3$-type structure (space group symmetry of *Pm3m* (No.221)). In the present work, we report the structural, electronic and elastic properties of these $REIn_3$ and $RETl_3$ (RE = Yb and Lu) compounds using density functional theory. A brief description of the computational details is outlined in Section 2 while Section 3 covers the results, followed by discussion.

2. Computational Method.

The present calculations are performed using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2k package [7]. The three different forms of generalized gradient approximation in the scheme of PBE-GGA [8], WC-GGA [9], PBE-sol GGA [10] are used for the exchange and correlation effects for the studied compounds. In order to achieve the energy eigen value convergence, we expand the basis function up to $R_{MT} \times K_{max} = 7$ where R_{MT} is the smallest atomic sphere radius in the unit cell and

K_{max} gives the magnitude of the largest *K* vector in the plane wave expansion. REX_3 compounds crystallize in the $AuCu_3$ structure with RE: 0, 0, 0; X: 0, 1/2, 1/2 (space group *Pm3m* (221). The total energies are calculated as a function of volume and fitted to Birch equation of state [11] to obtain the ground state properties. The elastic constants play an important role in determination of the strength, brittleness/ ductility and hardness of materials. In the present study, the elastic constants are calculated by using the method developed by Charpin and integrated incorporated in WIEN2k package [7].

The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. The symmetry of the cubic lattice reduces the 21 elastic constants to three independent elastic constants namely C_{11}, C_{12} and C_{44}. The elastic stability criteria for a cubic crystal at ambient conditions are $C_{11}+2C_{12} > 0$, $C_{44} > 0$ and $C_{11}- C_{12} > 0$ and $C_{12} < B < C_{11}$. The systems are fully relaxed after each distortion in order to reach the equilibrium state. C_{44} is proportional to the shear modulus and can be used as a measure of shear resistance.

3. Result and discussion

3.1. Ground state properties

The non-spin polarized electronic band structure calculations have been carried out to obtain the total energy of the $REIn_3$ and $RETl_3$ (RE = Yb and Lu) intermetallics using the first principles FP-LAPW method. In order to calculate the ground state properties, the total energies are calculated in $AuCu_3$ type structure for different volumes around the equilibrium cell volume V_0 using three different forms of generalized approximations (GGA) i.e. PBE-GGA, Wu-Cohen (WC) GGA and PBE-sol GGA. The calculated total energies are fitted to the Birch-Murnaghan equation of state [11] to determine the ground state properties like lattice constant (a_0), bulk modulus (B) and its pressure derivative (B') at minimum equilibrium volume V_0 using exchange correlation as PBE-GGA, Wu-Cohen (WC) GGA and PBE-sol GGA. The variation of total energy as a function of volume using PBE-GGA for these compounds is shown in Fig. 1 (a) – (d). It has been observed from E-V curves that all the studied $REIn_3$ as well as $RETl_3$ compounds are stable in non-magnetic phase.

The calculated ground state properties are given in Table 1, together with the available other theoretical calculations [5] and experimental data for comparison [12]. It is seen from Table 1 that our calculated values of a_0 are found to be in close agreement with the available experimental and other theoretical data. The bulk modulus of $LuIn_3$ is found to be highest, indicating that $LuIn_3$ is harder and least compressible compound as compared to other studied $REIn_3$ and $RETl_3$ compounds.

3.2. *Electronic properties:*

The calculated self consistent non-spin polarized electronic band structures (BS) along the high symmetry directions of $REIn_3$ and $RETl_3$ (RE = Yb and Lu) compounds using PBE-GGA in $AuCu_3$ phase are presented in Fig. 2 (a) - (d), where Fermi level is considered at zero. On the whole, the band profiles are seen to be almost the same in all the studied compounds except with slight variations in the position of highly localized '*f*' states of Yb and Lu. It is clear from all the band structures that all the studied non-magnetic compounds exhibit metallic nature. The lowest lying bands which lie in between -10.0 eV and -5.0 eV are due to '*s*' like states of X in YbX_3 and bands in between -10.0 eV and -6.0 eV in LuX_3 compounds are also due to X 's' like states of X. A flat band is observed near the Fermi level in valence band for YbX_3 are mainly due to '*f*' states of Yb whereas for LuX_3, it can be observed around -5.6 eV in valence band. There is hybridization of 's' and 'p' states of X with 'f' and 'd' states of RE at the Fermi level for all these compounds and are responsible for the strong metallic behavior. The cluster of bands above the Fermi level are due to the 'd' like states of RE and 'p' states of X. We have calculated the DOS at Fermi level N (EF) for these compounds and given them in Table 1.

3.3. Elastic properties

The elastic constants determine the response of the crystal to external forces, as characterized by bulk modulus, shear modulus, Young's modulus, and Poisson's ratio, and obviously play an important role in determining the strength and stability of materials. Elastic properties are also linked to sound velocity and Debye temperature. We have calculated the elastic constants of the $REIn_3$ as well as $RETl_3$ compounds in $AuCu_3$ structure using PBE-GGA as exchange correlation at ambient pressure using the method developed by Thomas Charpin and integrated it in the WIEN2k package [7]. The calculated values of elastic constants are given in Table 1. In the absence of any available measured data in the literature, these elastic constants could not be compared. It can be noted that our calculated elastic constants satisfy the stability criterions: $C_{11}- C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$,

$C_{12} < B < C_{11}$, which clearly indicate the stability of these compounds in $AuCu_3$ structure. We have also analyzed the ductility of all these compounds using Pugh's criteria. Our calculated result indicates that these compounds are ductile in nature. The elastic constants C_{11}, C_{12} and C_{44} increase linearly with pressure for all these compounds.

Conclusion

In conclusion, the structural, electronic and elastic properties of $REIn_3$ & $RETl_3$ (RE = Yb & Lu) have been studied by using the FP-LAPW method based on density functional theory within three different forms of GGA as exchange correlation potential. Our results on the structural, electronic, elastic and mechanical properties for these compounds are in agreement with available theoretical and experimental results. The ground state properties such as bulk moduli and lattice parameters are computed and compared with the preceding theoretical and other experimental results, which shows good agreement. The electronic properties of these compounds are studied by calculating band structures and its corresponding density of states. In present study, we found $B/G_H > 1.75$ for all the studied the compounds, which implies that all these compounds are ductile in nature We have calculated the second order elastic constants for the first time, which will be tested in the future experimentally and theoretically. Our calculated elastic constants obey the necessary mechanical stability conditions for cubic crystals.

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TABLE 1. Calculated ground state and electronic properties of $REIn_3$ and $RETl_3$ at ambient pressure.

Solid	Work	a_0 (Å)	B (GPa)	B′	$N(E_F)$ States/eV	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B/G_H
$YbIn_3$	PBE GGA	4.642	51.15	4.80	1.69	64.59	34.56	31.83	1.89
	WC GGA	4.543	57.86	5.20	1.57	-	-	-	-
	PBE-sol GGA	4.535	57.92	5.54	1.54	-	-	-	-
	Exp.	4.615[a]	-	-	-	-	-	-	-
	Other	4.594[b]	55.08[b]	4.40[b]	-	-	-	-	-
$LuIn_3$	PBE GGA	4.607	54.48	4.15	3.72	102.58	33.99	16.49	2.56
	WC GGA	4.520	64.42	3.88	3.55	-	-	-	-
	PBE-sol GGA	4.513	66.16	4.47	3.48	-	-	-	-
	Exp.	4.553[a]	-	-	-	-	-	-	-
	Other	4.566[b]	62.65[b]	4.16[b]	-	-	-	-	-
$YbTl_3$	PBE GGA	4.805	35.26	4.23	3.31	50.78	27.95	15.51	2.59
	WC GGA	4.687	47.13	3.51	3.53	-	-	-	-
	PBE-sol GGA	4.681	46.27	3.65	2.92	-	-	-	-
	Exp.	4.770[a]	-	-	-	-	-	-	-
$LuTl_3$	PBE GGA	4.739	53.25	4.41	2.23	54.81	41.11	23.04	3.22
	WC GGA	4.644	59.31	4.95	-	-	-	-	-
	PBE-sol GGA	4.637	59.15	4.50	-	-	-	-	-
	Exp.	4.653[a]	-	-	-	-	-	-	-

[a] Ref. [12], [b] Ref. [5]. Pre.- Present; Exp.- Experiment.

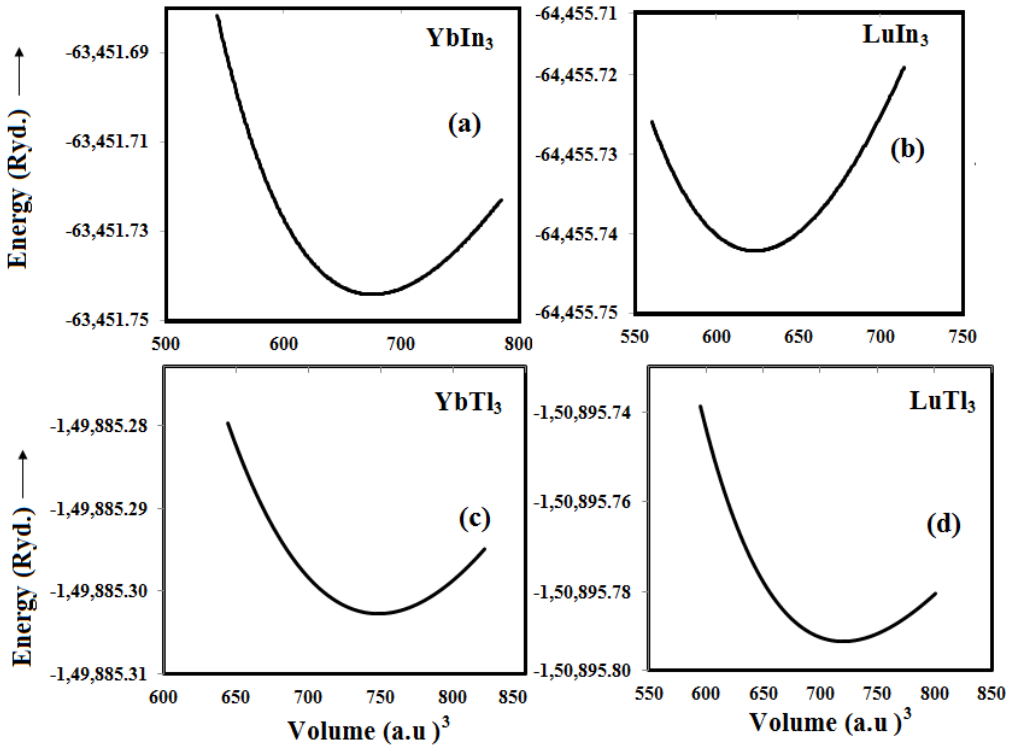

Fig. 1. Variation of total energy with the volume for $REIn_3$ and $RETl_3$ (RE = Yb, Lu) compounds.

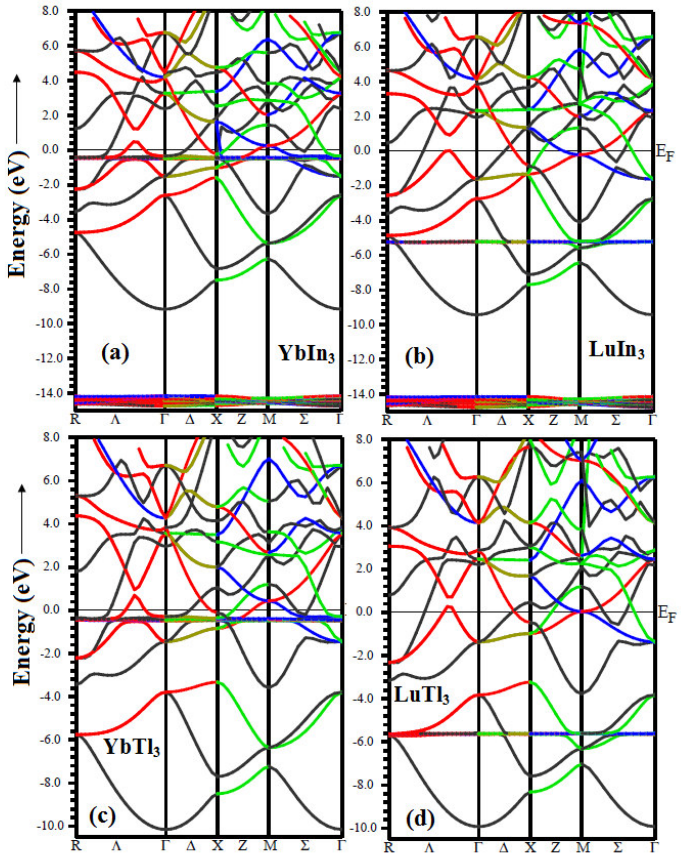

Fig. 2 (a) – (d). Band structure of $REIn_3$ and $RETl_3$ (RE = Yb, Lu) compounds at ambient conditions.

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