Structural, Electronic and Elastic Properties of Heavy Fermion YbTM$_2$ (TM= Ir and Pt) Laves Phase Compounds

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Abstract. The structural, electronic and elastic properties of YbTM$_2$ (TM = Ir and Pt) Laves phase intermetallic compounds which crystallize in cubic (MgCu$_2$-type) structure, have been investigated using ab-initio full potential linearized augmented plane wave (FP-LAPW) method with LDA and LDA+U approximation. The calculated ground state properties such as lattice parameter ($a_0$), bulk modulus (B) and its pressure derivative (B') are in good agreement with available experimental and theoretical data. The electronic properties are analyzed from band structures and density of states. Elastic constants are predicted first time for these compounds which obey the stability criteria for cubic system.

1. Introduction

AB$_2$ type Laves phase intermetallic compounds crystallize in three closely related structures namely cubic (MgCu$_2$) C15-type, hexagonal (MgZn$_2$) C14-type and di-hexagonal (MgNi$_2$) C36-type [1-2]. They are tetrahedrally closed packed layer structure in which A and B atoms are arranged in the maximum packing efficiency [3]. Laves phase compounds have received considerable attention in recent years as potential structural and hydrogen storage material. They have low density and high melting point [4]. There are many experimental and theoretical investigations have been done so far because of their verity of phenomena. The structural, electronic, elastic and magnetic properties of Laves phase compounds have been reported by several authors [5-9] using LDA and LDA+U method based on density functional theory. The specific heat of YbIr$_2$ at zero and applied magnetic field studied by Kim et al. [10]. The magnetic behavior of TmIr$_2$ and YbIr$_2$ has also observed by Willis et al. [11] using single crystal growth technique. The X-ray, micrographic analysis and magnetic measurement have been studied on Yb-Pt system and confirm that YbPt$_2$ consistent with MgCu$_2$ structure sequence in high temperature ranges by Iadelli et al. [12]. The neutron diffraction and magnetization measurement have been performed on PrX$_2$ (X = Ir, Pt, Rh and Ru) compounds for describe the magnetic properties [13].

In present paper, the structural, electronic and elastic properties of YbTM$_2$ (TM = Ir and Pt) Laves phase intermetallic compounds, which crystallize in cubic (MgCu$_2$) C15-type structure have been investigated using full potential linearized augmented plane wave (FP-LAPW) method with LDA and LDA+U approximation. There are no experimental and theoretical studies have been reported on electronic and elastic properties of YbTM$_2$ (TM = Ir and Pt) Laves phase compound in the literature so far.
2. Computational method
The YbTM$_2$ (TM = Ir and Pt) compounds crystallize in cubic MgCu$_2$-type structure with space group Fd$ar{3}$m (no. 227) [1]. The Yb and TM (Ir and Pt) atoms are positioned at (0.125, 0.125, 0.125) and (0.5, 0.5, 0.5) respectively [14]. All calculations have been carried out using full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k [15-16] code based on DFT. For exchange correlation, we have used the local density approximation (LDA) and LDA+U (U-Hubbard and exchange parameter) [17-18]. In our calculation we have used a $K_{max} \times R_{MT} = 7$ to obtain energy convergence, where $R_{MT}$ is the smallest atomic sphere radius in the unit cell and $K_{max}$ is the magnitude of the large $k$ vector in plane wave expansion. The partial wave value inside the atomic sphere is expanded up to $l_{max} = 10$ while in the charge density is Fourier expanded up to $G_{max} = 12$ (a. u.)$^1$. The core energy cut off is taken as -6.0 Ry. The calculations are performed with a dense mesh of $(9 \times 9 \times 9)$ $k$ points for both compounds and tetrahedral method [19] has been employed for Brillouin zone integration. The self-consistent calculations are converged when the total energy of system is stable within $10^{-4}$ Ry.

In the LDA+U method the effective parameter $U_{eff} = U - J$ where $U$ is coulomb interaction (Hubbard) parameter and $J$ is exchange parameter are taken to be different for different atoms of YbTM$_2$ (TM = Ir and Pt). The localized (4$f$-electrons) behavior resulted from electron correlation effects induced by the Coulomb interaction [20]. We use values of Coulomb interaction parameter $U = 7.5$ eV (Yb), 4.1 eV (Ir), 3.6 eV (Pt) and exchange parameter $J = 0.70$ eV for all elements. A good description of electronic properties of heavy rare earth based YbTM$_2$ compound is expected with LDA+U approximation because of presence of 4$f$ electrons in Yb ion and 4$f$-$5d$ electrons in transition metal (TM) ions.

3. Results and discussion
3.1 Structural and electronic properties
The non spin polarized calculations have been carried out to investigate the ground state properties of YbTM$_2$ (TM = Ir and Pt) Laves phase compounds. The total energy is calculated as a function of unit cell volume and fitted to Birch Murnaghan’s equation of state [21]. The energy versus volume curve has shown in figure 1 (a-b) and the calculated ground state properties such as lattice parameter ($a_0$), bulk modulus (B) and its pressure derivative (B’), which are listed in Table 1. with available experimental and theoretical results. The calculated values of lattice parameters are lower than the experimental Values of about 3% in LDA and LDA+U approximation.

Table 1. Calculated ground state and elastic properties of Laves phase YbTM$_2$ (TM = Ir and Pt) compounds.

| Solid   | Approximations | $a_0$ (Å) | B (GPa) | B' | $N(E_F)$ States/eV | C$_{11}$ (GPa) | C$_{12}$ (GPa) | C$_{44}$ (GPa) |
|---------|----------------|-----------|---------|----|-------------------|---------------|---------------|---------------|
| YbIr$_2$ | (LDA)          | 7.4051    | 237.02  | 5.22 | 10.10             | 326.51        | 202.99        | 160.75        |
|         | LDA+U          | 7.4173    | 231.38  | 4.00 | 3.52              | -             | -             | -             |
|         | Exp.           | 7.473$^a$ |         | 4.00 |                   | -             | -             | -             |
|         |                | 7.463$^b$ |         | 4.00 |                   | -             | -             | -             |
| YbPt$_2$ | (LDA)          | 7.4990    | 195.23  | 4.29 | 9.24              | 389.65        | 103.10        | 148.00        |
|         | LDA+U          | 7.5102    | 197.04  | 4.90 | 3.02              | -             | -             | -             |
|         | Exp.           | 7.545$^a$ |         | 4.90 |                   | -             | -             | -             |
|         |                | 7.546$^c$ |         | 4.90 |                   | -             | -             | -             |

$^a$Ref. [24], $^b$Ref. [10], $^c$Ref. [12]
It is also noticed that the calculated lattice parameters by LDA+U are slightly larger than the LDA. From Table 1, it can be seen that the bulk modulus of YbIr$_2$ is smaller than bulk modulus of YbPt$_2$, indicating that YbIr$_2$ is more compressible as compare to YbPt$_2$.

![Figure 1. Energy v/s Volume curves for YbIr$_2$ (a) and YbPt$_2$ (b) compound.](image1)

To elucidate the electronic properties of YbTM$_2$ (TM = Ir and Pt) Laves phase compounds we have calculated the electronic band structure, total and partial density of states by LDA+U approximation. The calculated band structure (BS) and DOS have shown in figure 2 and 3. It can be noticed that the nature of band structure for both compounds are almost similar. From figure 2, one can see that the Yb-4$f$ state is lying below the Fermi level as a flat band for both compounds. It shifts downward from the Fermi level with decreasing number of unpaired electrons in TM-5$d$ state because of weak interaction between Yb-4$f$ and TM-3$d$ in valence region [7]. The lowest lying bands are mainly due to

![Figure 2. Electronic band structure for YbIr$_2$ (a) and YbPt$_2$ (b) compounds from LDA+U approximation.](image2)
3$d$-like state of transition metal (TM = Ir and Pt) which can be seen from Figure 2 in energy range -4.8 to -1.4 eV and -5.4 to -2.4 eV for YbIr$_2$ and YbPt$_2$, respectively. In the conduction region the 5$d$- state of transition metal (TM = Ir and Pt) is hybridize with Yb-5$d$ state near the energy range 4 eV for both compounds. We have calculated the DOS at Fermi level for both of the compounds and are presented in Table 1. The DOS at Fermi level is clearly show the metallic nature of both compounds. It is also seen from figure 3, the highest peak is create by Yb-4$f$ state. The 5$d$- state of TM give maximum contribution in DOS figure as interaction with Yb-4$f$ and 5$d$-state in valence and conduction region respectively.

### 3.2 Elastic properties

The elastic constants provide important information about stability, stiffness of materials and nature of interatomic forces. We have calculated the elastic constants of YbTM$_2$ intermetals, at ambient pressure by using the method developed by Charpin [22]. A cubic structure has three independent elastic constant namely $C_{11}$, $C_{12}$ and $C_{44}$. The calculated values of elastic constant satisfy the Born-Huang criterions for stability: $C_{11} - C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$ [23] and are given in Table 1. The elastic constants have calculated first time for the studied compounds, hence there are no theoretical and experimental data exist in literature for comparison.

### 4. Conclusion

In this work we have used first principles calculations using the FP-LAPW method within the LDA and LDA+U approximation to describe the structural, electronic and elastic properties of Laves phase YbTM$_2$ (TM = Ir and Pt) compounds. The calculated lattice parameters are in good agreement with the available experimental data. The electronic band structures confirm the metallic nature of YbTM$_2$ (TM =Ir and Pt) Laves phase compounds. The calculated elastic constants satisfy the stability criteria.

### Acknowledgement

The authors are thankful to Nikita Acharya and Deepika Shrivastava for useful discussions and help in computations.
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