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Physical Properties of Yttrium-Rhodium and Yttrium-Copper B2-Type Rare Earth Intermetallic Compounds: First Principles Study

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Abstract

The electronic structure of B2-YCu and YRh intermetallic compounds which crystallize in the CsCl structure has attracted the attention of the scientific world because of their excellent mechanical properties. The advantage of studying these materials is to answer of some industrial request in the materials that resist for high temperature and high oxidation resistance. However, high ductility has been observed in these compounds at room temperature. In this present work, we employed ab initio calculation methods while basing on the full-potential linearized augmented plane wave (FP-LAPW) method within density functional theory implanted in the Wien-2 k code, which is used to examine the various properties of these materials (YCu, YRh) like structural, electronic, and elastic properties. The results obtained are in good agreement with those found in other theoretical studies and experimental data.

Keywords: intermetallic compounds, electronic structure, elastic properties, FP-LAPW method

1. Introduction

The intermetallic compounds typically possess chemical, physical, and mechanical properties superior to those of ordinary metals. They have many applications in engineering due to their high melting points, high tensile strength, good stiffness, low density, high corrosion, and oxidation resistances at elevated temperature [1, 2]. However, the brittle comportment and low ductility of these intermetallics at ambient temperature severely limit their application.

The previous studies revealed that the brittleness of intermetallic systems increases when the symmetry of the unit cell decreases and the number of atoms by unit cell increases [3]. In 2003, it has been discovered by scientists at Ames Laboratory (Iowa University) that a new type of binary stoichiometric rare earth intermetallic compounds possesses high ductility at room temperature [4–6]. They have B2 CsCl-type structure with equal atomic ratios and have R-M formula, where R is the rare earth and M is the transition metal. YCu and YRh are typical members of this family of B2 ductile rare earth intermetallics. Furthermore, many experimental and theoretical works have examined these compounds. The phase stability, elastic constants, and electronic structure of YCu have been recently studied by ab initio calculations [7–9]. The electronic properties of YCu and YRh were calculated by Khadeer et al. [10] utilizing TB-LMTO technique. The crystal-field (CF) parameters and electronic structure of YRh and YCu crystals were calculated by Divis and Kuriplach [11]. In the last years, an ab initio study of structural, elastic, and electronic properties of YRh has been reported in Refs. [12–14]. The dissociation and core properties of dislocations in YCu were investigated by using the generalized Peierls-Nabarro formalism [15]. The ductility mechanism of YCu and YRh has been determined in Ref. [12]. Chouhan et al. [16] have also studied the electronic, thermo-elastic, and mechanical properties of YCu. The rare earth ions in intermetallic compounds are generally trivalent [17]. The result indicates that YRh has more significant ductility than YCu. To understand some of the physical properties of these compounds, the electronic structures of these compounds are required. In this chapter, we present ab initio calculations of the properties of YRh and YCu compounds, including the structural parameters, elastic constants, band structure, and density of state (DOS), which are computed and compared with the available theoretical and experimental results.

2. Methodology

In this work, we have employed the full-potential linearized augmented plane wave (FP-LAPW) method [18, 19] as implanted in the Wien-2 k code developed by Blaha et al. [20]. The exchange and correlation effects are described in the framework of the density functional theory with the parameterization of Perdew et al. [21]. To confirm the convergence of our calculations, we carefully investigate the dependence of total energy of the cutoff energy and the k-point set mesh according to the Monkhorst pack grid [22]. The unit cell is divided into no overlapping muffin-tin spheres of radius R_{MT} and an interstitial region, where the Kohn-Sham wave functions are expressed in spherical harmonic functions within spheres and plane waves in the remaining space of unit cell. We use the value of $R_{\text{MT}} K_{\text{max}}$ equal to 8 which determines the matrix size, where K_{max} is the PW cutoff and R_{MT} is the muffin-tin radius. Basis functions, charge density, and potential were expanded inside the muffin-tin spheres in spherical harmonic functions with cutoff $l_{\text{max}} = 10$ and in Fourier series in the interstitial region. The iteration process was repeated until the calculated total energy of the crystal converged to less than 0.5 mRy/unit cell. A mesh of 35 special k-points is used in the irreducible wedge of the Brillouin zone. We have taken the R_{MT} for Y, Cu, and Rh equal to 2.0, 1.87, and 2.3 a.u., respectively. YRh and YCu crystallize in the B2 CsCl-type structure with space group $\text{Pm}\bar{3}\text{m}-N^{\circ} 221$, where Rh and Cu atoms are occupied $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ position and Y occupy $(0, 0, 0)$ position. The following basic orbital is used:

Y: $5s^2, 5p^0, 4d^1$

Cu: $4s^1, 3d^{10}, 4p^0$

Rh: $5s^2, 5p^0, 4d^8$

3. Lattice parameters and elastic properties

As a first step, the total energy of YCu and YRh was calculated at many different volumes around equilibrium fitted to Murnaghan's equation of state [23] from which we obtained the equilibrium structural parameters. This is performed by applying hydrostatic pressure by changing the lattice parameters while keeping the c/a and b/a ratios constant with the optimized volume. The variation of the total energy with the relative volume for YCu and YRh compounds is given in **Figure 1(a, b)**. The calculated equilibrium lattice parameter and the bulk modulus of each of these compounds, which are in the B2 structure, are compared with the available experimental data and some theoretical results. They are tabulated in **Table 1**. The calculated lattice parameters and the bulk modulus (B) for YCu are in good agreement with those measured experimentally. Hence, we can conclude that the computation parameters and conditions selected in the present work should be suitable. The calculated values of the Bulk modulus (B) are 70.149 and 108.507 GPa for YCu and YRh compounds, respectively, indicating a disagreement with those found by Khadeer and coworkers [10] which indicates values of 97.49 GPa for YCu and 49 for YRh obtained by TB-LMTO method within the atomic sphere approximation (ASA). The difference is essentially due to the fact that they used the LDA approximation with relativistic effect, while we have used the GGA approximation. So, there are no experimental results available to us for YRh compounds. We have also calculated the elastic constants (C_{11} , C_{12} and C_{44}) in B2 phase at the equilibrium volume for these cubic compounds using the method discussed in detail in Ref. [28]. In all cases the comparison is quite agreeable. The largest

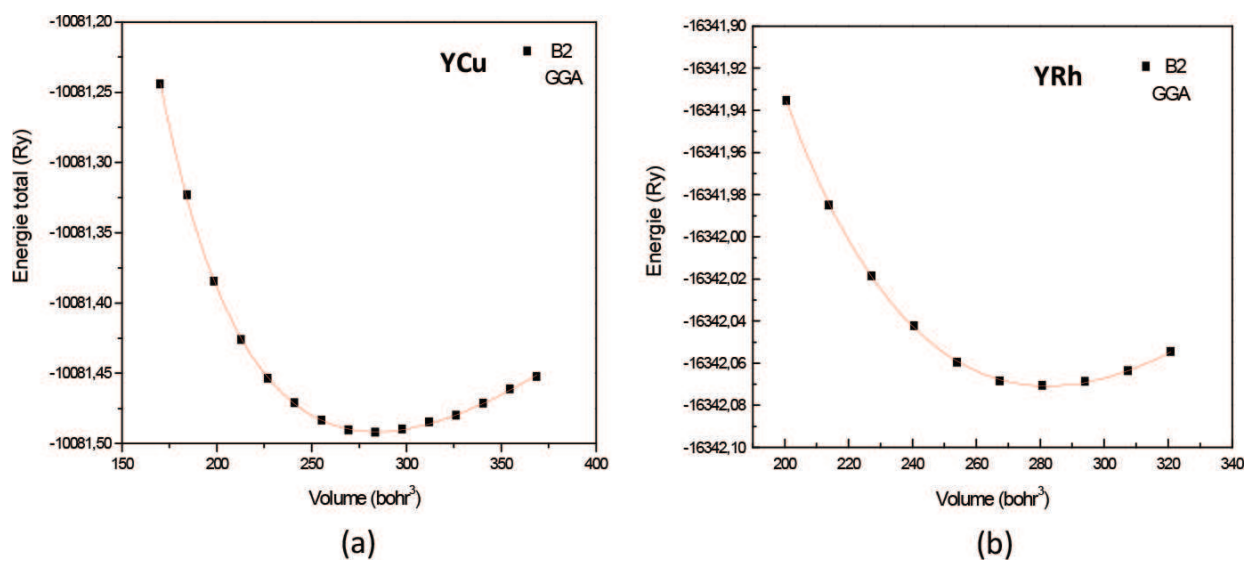


Figure 1. Calculated total energies as a function of volume in B2 phase for YCu (a) and YRh (b).

	YCu			YRh		
	Present	Exp.	Other theories	Present [14]	Exp.	Other theories
a_0 (Å)	3.47	3.477 [7]	3.475 [24], 3.418 [10], 3.478 [16]	3.47	3.408 [11], 3.415 [12]	3.368 [12], 3.43 [13]
B (GPa)	70.14	70.1 [7], 70.0 [25]	97 [10], 70 [7], 70 [25], 69.8 [16]	108.50	/	113.4 [12], 115.78 [13], 49 [10]
C_{11} (GPa)	116.94	113.4 [7]	117.7 [26], 113.6 [12], 116 [7], 114.4 [25], 121.9 [16]	133.48	/	171.0 [12], 186.47 [13]
C_{12} (GPa)	46.43	48.4 [7]	47.2 [26], 48.4 [12], 47 [7], 47.8 [25], 49.1 [16]	96.01	/	83.6 [12], 80.44 [13]
C_{44} (GPa)	32.05	32.3 [7]	36.1 [26], 36.8 [12], 35 [7], 34.3 [25], 35.7 [16]	20.14	/	38.4 [12], 51.64 [13]
G (GPa)	33.33	32.38 [27]	35.25 [26], 35.9 [16]	19.57	/	/
B/G	2.10	2.140 [7]	1.977 [26], 1.944 [16]	5.54	/	/
A	0.90	0.99 [7]	1.02 [26], 0.98 [16]	1.07	/	/
ν	0.284	0.299 [7]	0.286 [26], 0.289 [16]	0.41	/	/
E (GPa)	133.333	85.1 [16]	91.80 [26], 92.7 [16]	78.31	/	/

Note that the values of our calculations are given at $T = 0$ K values, while the experiments are given at room temperature.

Table 1. Lattice parameter and elastic constants (C_{ij}) for YCu and YRh compounds. The bulk modulus (B), shear modulus (G), elastic anisotropy (A), Poisson's ratio (ν), Young's modulus (E) and available experimental values are also given.

discrepancy between theory and experiment is the value for C_{12} for YCu, where the difference is approximately 4.24%. The value for C_{11} is also different by 3%. Our calculated positive value of the elastic constants ($C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$, and $C_{11} + 2C_{12} > 0$) is an indication of the mechanical stability of YCu and YRh. There are no experimental results available to us for YRh compound. We hope that our present work will stimulate some more works in the YRh compound.

In addition, the elastic constants are correlated to numerous macroscopic parameters as the shear modulus (G), Young's modulus (E), Poisson's ratio (ν), and the elastic anisotropy (A). The results obtained by our method (FP-LAPW) of calculation are presented in **Table 1**, including the experimental data and those obtained by other numerical approaches.

The polycrystalline shear modulus is associated with the resistance to plastic deformation, while the bulk modulus represents the opposition to band rupture. The polycrystalline shear modulus is described by equation [7]:

$$G = \frac{C_{11} - C_{12} + 3C_{44}}{5} \quad (1)$$

as well as the bulk modulus (B) is given by the following equation:

$$B = \frac{C_{11} + 2C_{12}}{3} \quad (2)$$

Young's modulus expresses the rigidity of the material. For a cubic structure, it is related to the shear modulus and bulk modulus by [29]

$$E = \frac{9BG}{3B + G} \quad (3)$$

The relation between Poisson's ratio and the elastic constants is expressed by

$$\nu = \frac{C_{12}}{C_{11} - C_{12}} \quad (4)$$

It is well known that microcracks are easily induced in the material due to the significant elastic anisotropy. Hence, it is very important to calculate the elastic anisotropy factor (A) in order to improve their mechanical durability. The elastic constants can be described by the following expression [7]:

$$A = 2 \frac{c_{44}}{c_{11} - c_{12}} \quad (5)$$

The elastic constants (C_{ij}) permit calculation of Pugh's factor [30] for these materials investigated here. Pugh proposed that for materials with melting temperature above 900°C, the bulk modulus (B) divided by the shear modulus (G) predicts whether the material is expected to deform in a ductile or brittle manner: if $B/G > 1.75$, then the ductile behavior is predicted, else the materials have brittle behavior. Therefore, using the relation between the bulk modulus (B), shear modulus (G), and the elastic constants (C_{ij}), the ratio B/G can be calculated for RM ($M = \text{Cu}$ and Rh). From **Table 1**, the value of Pugh's factor (2.104) for YCu is consistent with the recent theoretical and experimental studies.

The calculated Poisson's ratio (ν) and the anisotropy constant (A) are also given in **Table 1**. For YCu, one can observe that the calculated value of the elastic anisotropy (A) is inferior to the experimental value [7]; the error is around 8%. For Poisson's ratio (ν), we find a good agreement with the theoretical studies and the experimental data. The values of anisotropy factor calculated are close to unity signifying that the YCu and YRh studied have isotropic elasticity.

In **Table 1**, we also observed that the YCu material has a low bulk modulus (70.149 GPa) and a relatively low B/G ratio (2.104), which reflects a high value of shear modulus (G). As a result, YCu undergoes a lower deformation than YRh compound. YRh is more ductile than YCu (due to the relatively low shear modulus (19.578 GPa) and high bulk modulus (108.507 GPa)) and has less rigid structure ($E_{(\text{YRh})} < E_{(\text{YCu})}$). This tendency underlines proportionality found between the toughness and the ductility.

4. Band structure calculation and density of state (DOS)

In this section, it is interesting to examine the electronic structure for YCu and YRh compounds at equilibrium volume using the accurate full-potential linearized augmented plane

wave (FP-LAPW) method with PBE-GGA approximation. The calculated band energies along the higher symmetry directions are presented in **Figure 2**. It can be seen that both materials possess a large dispersions of the free electrons around Γ point and an overlap of the bands, which confirm us the metallic character. The overall band profiles obtained in the present work are in fairly good agreement with the tight-binding linear muffin-tin orbital (TB-LMTO) calculations [10, 11] using the LDA approximation. In **Figure 2a**, the bands in the energy domain between -4 and -2 eV are largely predominant by the d states of the Cu atom. The bands near the Fermi energy (E_F) are due to Y-d states. Some bands lying around -3.0 eV, following along the direction $+\Gamma$ are nearly flat, indicating that the recovery of the orbital between the neighboring atoms is more restricted, and other bands of high energy that are around 4.0 eV present a large dispersion. For YRh, below the Fermi energy, the bands are predominantly by Rh-d states, while at high energies, one can find bands due to Y-d states. A pseudo-gap was also observed at the Fermi energy level. The bands are narrow. They are characterized by a doubly degeneration of bands in the point Γ ; it is due to the cubic symmetry of crystals (**Figure 2b**).

The density of state (DOS) for YCu and YRh compounds is calculated in B2 phase by the method of the standard tetrahedron [29]. The total and partial densities of states have also been plotted for both YCu and YRh and are shown in **Figures 3** and **4**, respectively. From these figures, the following observations have been made. For YCu, we find that the large occupied peak is located at energy range between -6.0 and -1.9 eV in valence region, which is dominated by Cu-d state below the Fermi energy ($E_F = 0.621$ eV). In the

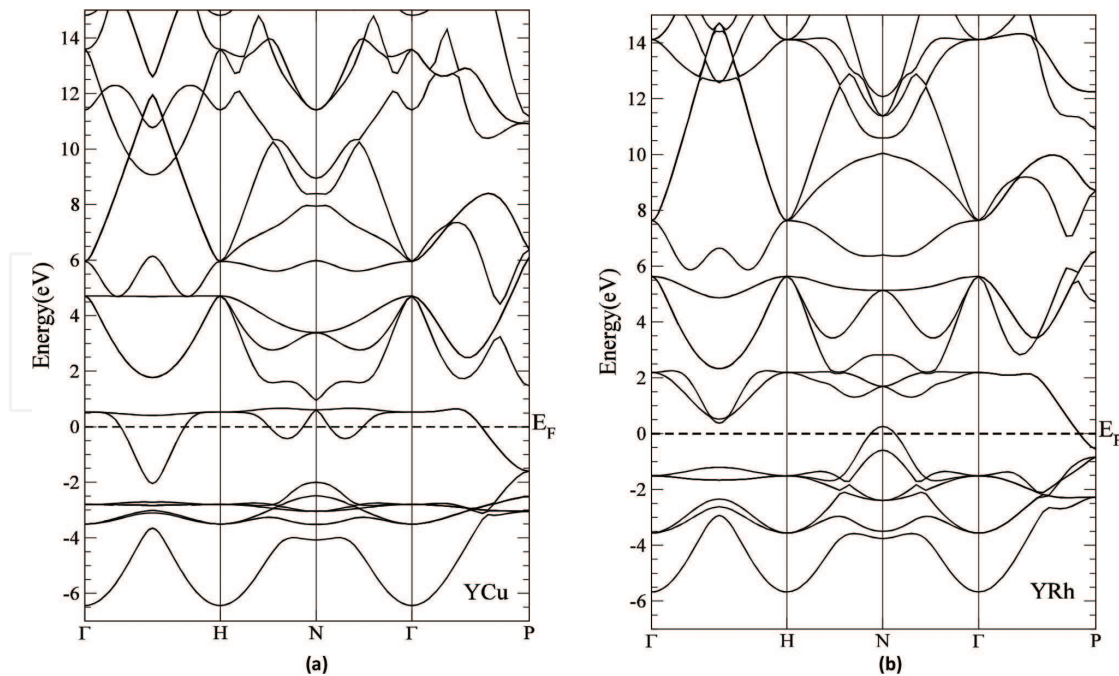


Figure 2. Band structure for YCu (a) and YRh (b) in B2 phase.

conduction band above the Fermi level, the states are mainly due to Y-d state. The DOS of YRh (Figure 4) is similar to YCu, while the large occupied peak is dominated by the Rh-d state in the valence band (states below the Fermi level $E_F = 0.773$ eV). At higher energy around 4 eV, one can find DOS mainly due to Y-d states. The location of the Fermi level near a local minimum in the DOS is very important for the stability of these binary rare earth intermetallic compounds. We have also observed that the densities of states at the Fermi level $N(E_F)$ are different to zero which indicates the metallic character for YRh and YCu.

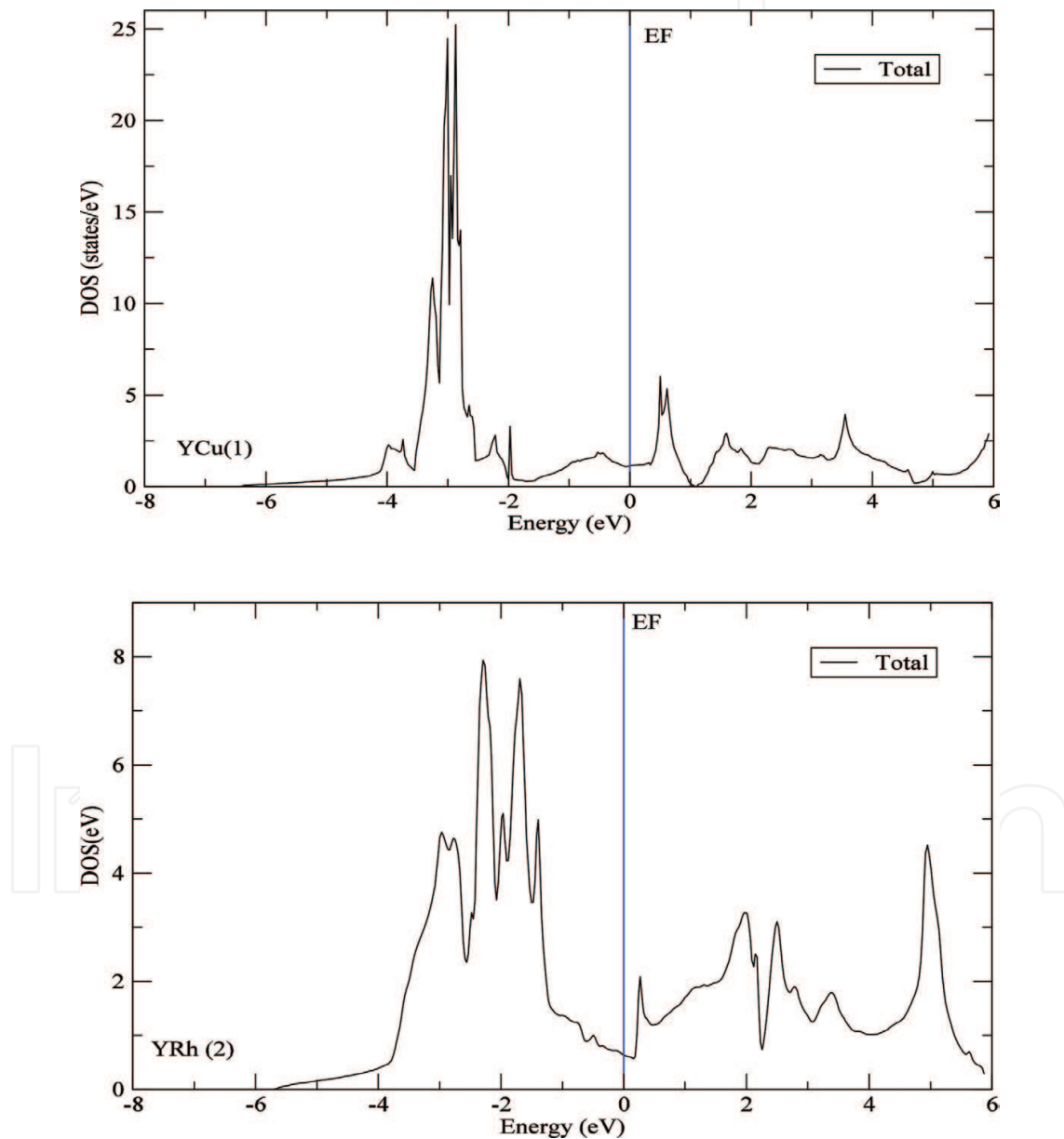


Figure 3. Total densities of states of YCu (1) and YRh (2) in the B2 structure.

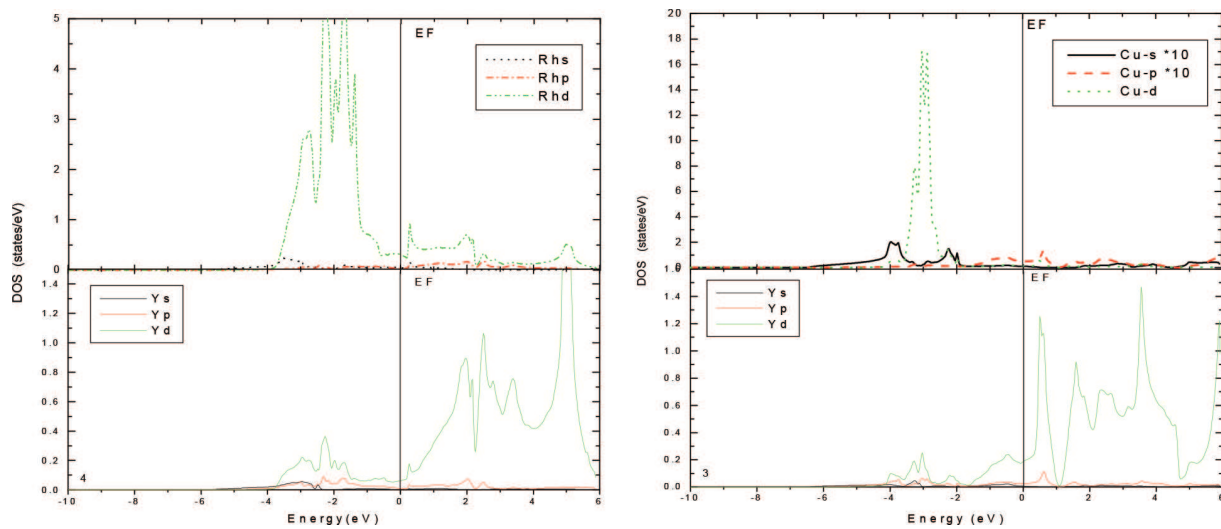


Figure 4. The partial electronic densities of YCu (1) and YRh (2) in the B2 structure.

5. Conclusion

In this chapter, we have investigated the structural, electronic, and elastic properties of YCu and YRh B2 rare earth intermetallics by means of the full-potential linearized augmented plane wave (FP-LAPW) approach. The use of the PBE-GGA approximation for the exchanging correlation potential allowed us to obtain good values of the electronic structure. The value of the bulk modulus obtained in YRh material is in disagreement with those found by the method TB-LMTO. This difference can be justified later by the experience. Our calculations demonstrate that the YM ($M = \text{Cu}$ and Rh) ductile materials are significantly different than previously studied intermetallic B2 compounds. The elastic constants have significantly more isotropic behavior, and Poisson's ratio is smaller than theoretical value (<0.25) indicating that these materials are compressible. The calculated band structure and density of state (DOS) were in good agreement with other theoretical calculations. The remarkable characteristic is that the total density of state (DOS) of these B2 rare earth intermetallics is similar. In addition, there are no experimental studies on the bulk modulus and elastic properties of YRh compound. Hopefully, these results will encourage further experimental works on YRh intermetallics to test and refine the theoretical works. So, it may be interesting to perform high-pressure X-ray diffraction studies on this compound.

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