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Metallic behaviour at YBaCuO7/Zas interfaces (G=Ga, Al)

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We present the electronic band structure of the interfaces $YBa_2Cu_3O_7$/GaAs (direct gap) and $YBa_2Cu_3O_7$/AlAs (indirect gap) in different configurations calculated using the Density Functional Theory as in the Wien2k code within the local density approximation. We have projected the density of states at the atomic layers forming the interface. We concentrated on the semiconductor side. The four first atomic layers in the semiconductor side of the interface present a clear metallic behaviour. We found for both semiconductors considered that it converges towards the bulk atomic-layer projected density of states a few atomic layers from the interface. We considered an ideal non-reconstructed interface in the (001) direction first and let it relax using the corresponding option in the Wien2k code. The behaviour does not change in an important way and we found but small deviations from the ideal case in the Density of States of the relaxed interface. It is important to relax the interface since the metallic behaviour of the semiconductor side of the could have been suppressed which is the most interesting result of this work. The behaviour at the interface is interesting and could be used in several technological applications and it opens, for example, the possibility to induce superconductivity on the semiconductor side of the metal/semiconductor interface.

Keywords: YBaCuO7; semiconductors; interfaces; electronic structure.

PACS: 31.15.E-; 73.20.-r; 73.61.Ey; 74.72.-h

1. Introduction

There are several electronic applications with Superconductor/semiconductor interfaces including, for example, amplifier hybrid circuits [1], hybrid transistors [2], magnetic micro-switches [3], light-emitting diodes [4], diode-detectors [5] and memories [6,7], among others [8,9]. The possible change of character at the semiconductor side of a superconductor/semiconductor interface, could allow the semiconductor well established technology to take advantage of the known properties of superconductors for technological applications.

$YBa_2Cu_3O_7$ is a second generation superconductor with a critical temperature of the order of 90 K [10]. Interfaces containing this superconductor and metals have been studied experimentally [11-13] as well as theoretically [14-16] since long ago. Nevertheless, the superconductor/semiconductor interfaces have been scarcely studied except for some oxides [17,18].

In general, the change of character at an interface is of interest. A metallic behavior in semiconductors, for example, has been obtained at a semiconductor/semiconductor interface [19] by introducing vacancies. The metallic behavior at the semiconductor side of a superconductor/semiconductor interface could induce superconductivity at the semiconductor side. This would open the possibility that the nano-circuit technology that has been intensely developed for semiconductors can be employed with the advantage of the superconducting behavior since no heat will be produced. To induce superconductivity in a semiconductor is not new idea. It has been discussed long ago by Marvin Cohen [20,21], for example. Also, interfaces with semiconductors as one of the components are of interest in spintronics and spin polarized transport [22].

2. Computational Details

We use in our calculations the Density Functional Theory (DFT) [23,24] with Linearized Augmented Planes Waves plus local orbitals (LAPW+lo) [25] as implemented in the Wien2k code [26] together with the Local Density Approximation (LDA). In a run $YBa_2Cu_3O_7$/GaAs, we used the Generalized Gradient Approximation (GGA) instead but found no significant differences. We used a cut-off $R_{\rm mt}K_{\rm max} = 7.0$, a Muffin-tin radius, $R_{\rm mt}$, equal to 2.3 for Y, 2.5 for Ba, 1.79 for Cu, 1.58 for O, and 2.22 for Ga, Al and As in atomic units, when in the configuration shown in Fig. 1a. When in the configuration shown in Fig. 1b and Fig. 1c, $R_{mt} = 2.2$ a.u. in the first atomic layer (either Ga, As or Al) and $R_{mt} = 2.0$ a.u. for the second layer (either Ga, As or Al). We take YBCO7 in the normal state.

The lattice matched ideal interfaces were built up with two unit cells of the semiconductor and one of the superconductor which acts as the substrate and therefore the semiconductor takes the lattice parameter of the YBCO7. To avoid tension at the interface as much as possible we have turn the semiconductor unit cell by 45° around the z-axis. We considered orthorhombic $YBa_2Cu_3O_7$ (spatial group $Pmmm$), with lattice parameters [28] $a = 3.823$, $b = 3.886$, $c = 11.681$ in Å. The semiconductor is therefore under tension in the way shown in Table I. The new lattice parameters for the semiconductor ($a_\parallel$ and $a_\perp$) differ from the original ones ($l_{\rm GaAs} = 5.653$ Å, $l_{AlAs} = 5.660$ Å) and were calculated in the following way. The x and y axis parameters

TABLE I. Parameters used in the calculation for the semiconductors.

Semiconductor	GaAs	AlAs
Lattice constant of the bulk l_j (Å)	5.653	5.660
Parallel lattice constant $l_{j\parallel}$ (Å)	5.452	5.452
Perpendicular lattice constant $l_{j\perp}$ (Å)	5.876	5.882
Stress on $l_{j\parallel}$ (%)	3.57	3.70
Stress on $l_{j\perp}$ (%)	3.94	3.90
Elastic constant in GPa [29]		
C_{11}^j	118.4	125
C_{12}^j	53.7	53.4

(parallel to the a and b axis of the superconductor) are given by

$$l_{j\parallel} = \sqrt{a^2 + b^2} \tag{1}$$

In the z-direction, the semiconductor lattice parameter is given by [27]

$$l_{j\perp} = (1 - \sigma_{ST} f_j) l_j \tag{2}$$

where

$$\frac{\Delta l_j}{l_j} = \frac{l_j - l_{j\parallel}}{l_j} = -f_j. \tag{3}$$

The σ_{ST}^j parameter is

$$\sigma_{ST}^j = \frac{C_{11}^j}{2C_{12}^j} \tag{4}$$

C_{11}^j and C_{12}^j are the elastic constants of the semiconductor.

3. Interfaces Considered

We have performed the calculation of the Interface Density of States (IDOS) for the following systems,

1. CuO-chains terminated $YBa_2Cu_3O_7$ with both Ga (As) terminated GaAs rotated 45° clockwise so that the first atomic layer on the semiconductor side faces the sides of $YBa_2Cu_3O_7$ that do not contain oxygen atoms (see Fig. 1a). We label the interfaces accordingly as chain/X, X=AsGa (meaning that the As atomic layer is facing $YBa_2Cu_3O_7$), chain/GaAs, chain/AlAs and chain/AsAl. We took the distance between the adyacent atomic layers (d) at the interface as $d = (d_1 + d_2)/2$ where d_1 and d_2 are the distance between the two first atomic layers at each side of the interface.

2. Same system but now the rotation of the semiconductor is counter clockwise so that the atoms on the first atomic layer of the semiconductor side face the oxygen atoms of the superconductor chains We denote them as chain$_O$/X, where X has the same definition as before (See Fig. 1b). We took the distance at the interfaces as $d = 2.0$ Å so that all core states lie inside the muffin-tin sphere.

3. The third series of calculations were performed with CuO_2-plane terminated $YBa_2Cu_3O_7$, which we denote as plane/X where X is defined as before. The rotation was made clockwise. The calculation with the rotation counter clockwise was not performed since the difference in the resulting position of the O-atoms is very small (a 0.06% difference with respect to the YBCO7 c-axis length). (See Fig. 1c). We took the distance at the interfaces as $d = 2.2$ Å so that all core states lie inside the muffin-tin sphere.

4. Results and Discussion

We present in Fig. 2, the Interface Density of States (IDOS) obtained in all the cases considered in this work. A very remarkable result is that in all the configurations considered the first few layers in the semiconductor side present a metallic behavior. This change of character might turn out to be very usefull in technological applications. In more detail, we obtained three somehow different results presented below. In Fig. 2a, we present the IDOS projected on the first two atomic layers of the interface chain/AsGa. The major contribution in these two layers comes from states of p-symmetry. The Fermi energy is at the origin. As it is apparent from the figure, the two atomic layers from the semiconductor side facing the chains of YBCO7 present a metallic behavior. In Fig. 2b, we present the first two atomic layers of the chain/GaAs. Here again we can see that the two atomic layers are metallic. In Fig. 2c, we present the IDOS for the two first atomic layers on the semiconductor side for plane/GaAs interface.

In general, our results show that all the interfaces of the form chain/AsZ, chain$_O$/AsZ and plane/AsZ behave as show

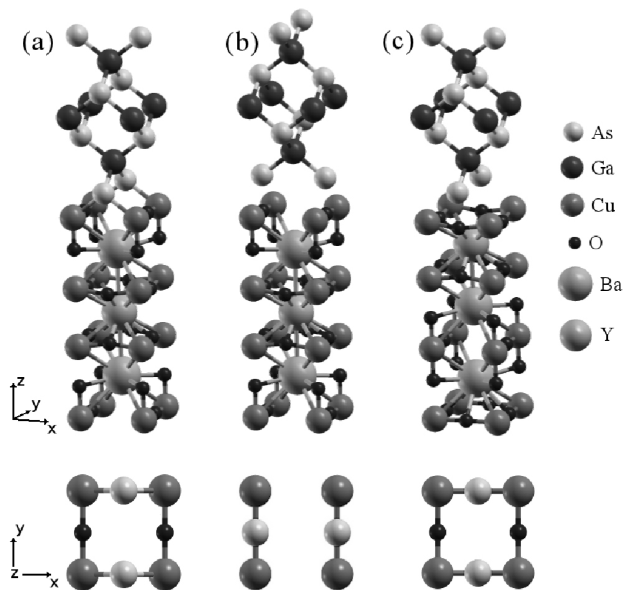

FIGURE 1. The interfaces studied a) chain/X, b) chain$_O$/X and c) plane/X. See text for the definition of the symbols.

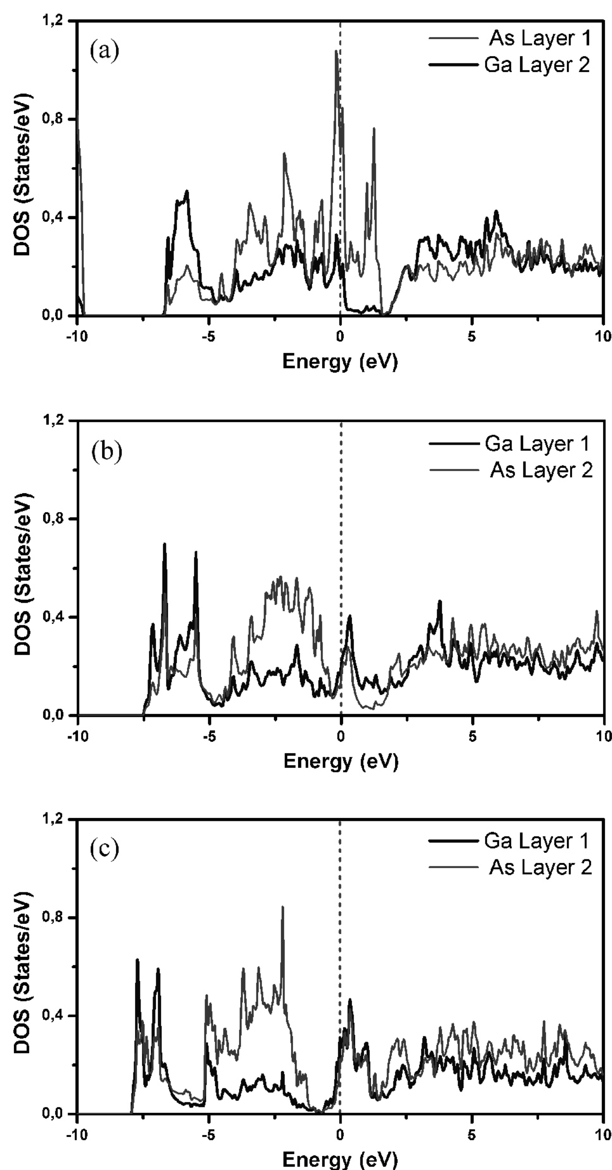

FIGURE 2. Results for the interfaces a)chain/AsGa, b)chain/GaAs and c)plane/GaAs.

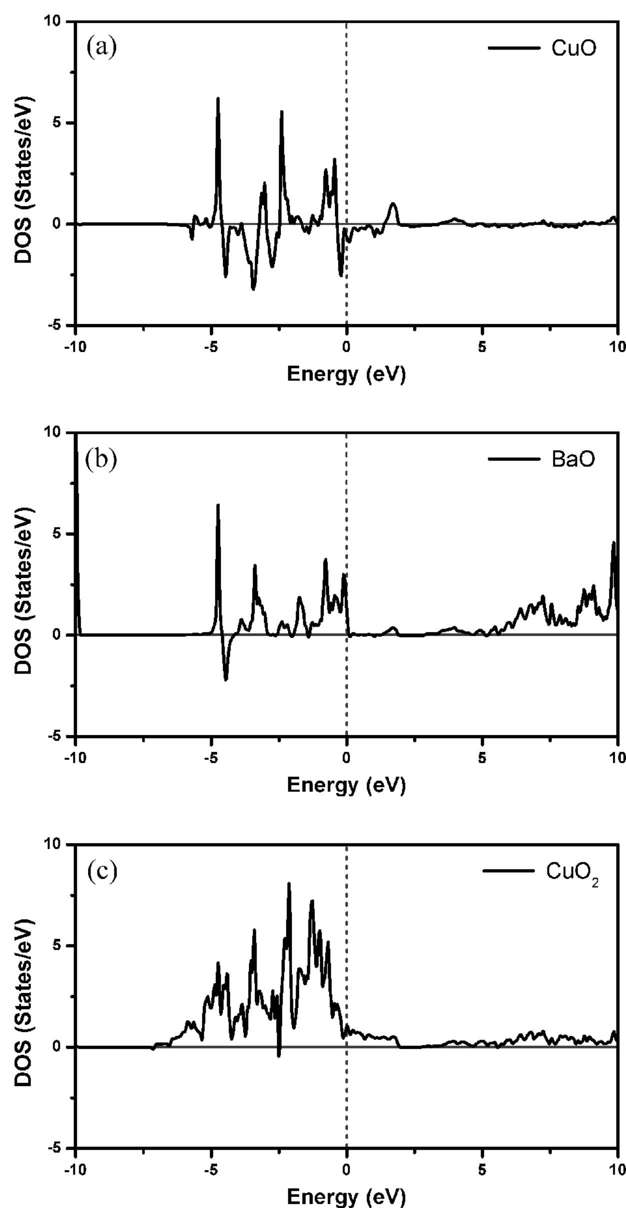

FIGURE 3. Difference between the bulk YBCO7 atomic-plane Local Density of States (LDOS) and the IDOS at the same atomic plane for the chain/AsGa case. (a)CuO, (b) BaO and (c) CuO_2.

shown in Fig. 2a, the interfaces of the kind chain/ZAs, chain_O/ZAs behave as illustrated in Fig. 2b and the interfaces plane/ZAs behave as illustrated in Fig. 2c.

Since at thermal equilibrium the Fermi level is unique for the two sides of the interface, electron states are redistributed. We illustrate this in Fig. 3. The Atomic-Plane Local Density of States (LDOS), is compared to the corresponding Bulk LDOS. We present in Fig. 3 the difference (Bulk-Interface) between the two to show explicitly the changes at different frequencies.

In Fig. 3, we present the difference at the CuO-plane (Fig. 3a), the planes BaO (Fig. 3b), and CuO_2 (Fig. 3c). The CuO_2 plane looses charge the most, as it is evident from Fig. 3c. Looking in more detail, oxygen in both, the CuO and the CuO_2 planes looses about the same amount of charge. The Cu atoms at these planes loose the most while the Ba atoms and the BaO planes loose almost nothing and seem not to be most influenced by the interface. This is common to all the different interfaces studies for both, the chain or plane interfaces.

At the semiconductor side, charge redistribution renders metallic several atomic planes. As the plane distance from the interface enhances, its LDOS recovers the bulk LDOS and the material becomes a semiconductor again. This is illustrated in Fig. 4a.

5. The effect of relaxation

It is important to relax the interface so as to check that the results presented above are not qualitatively modified. We

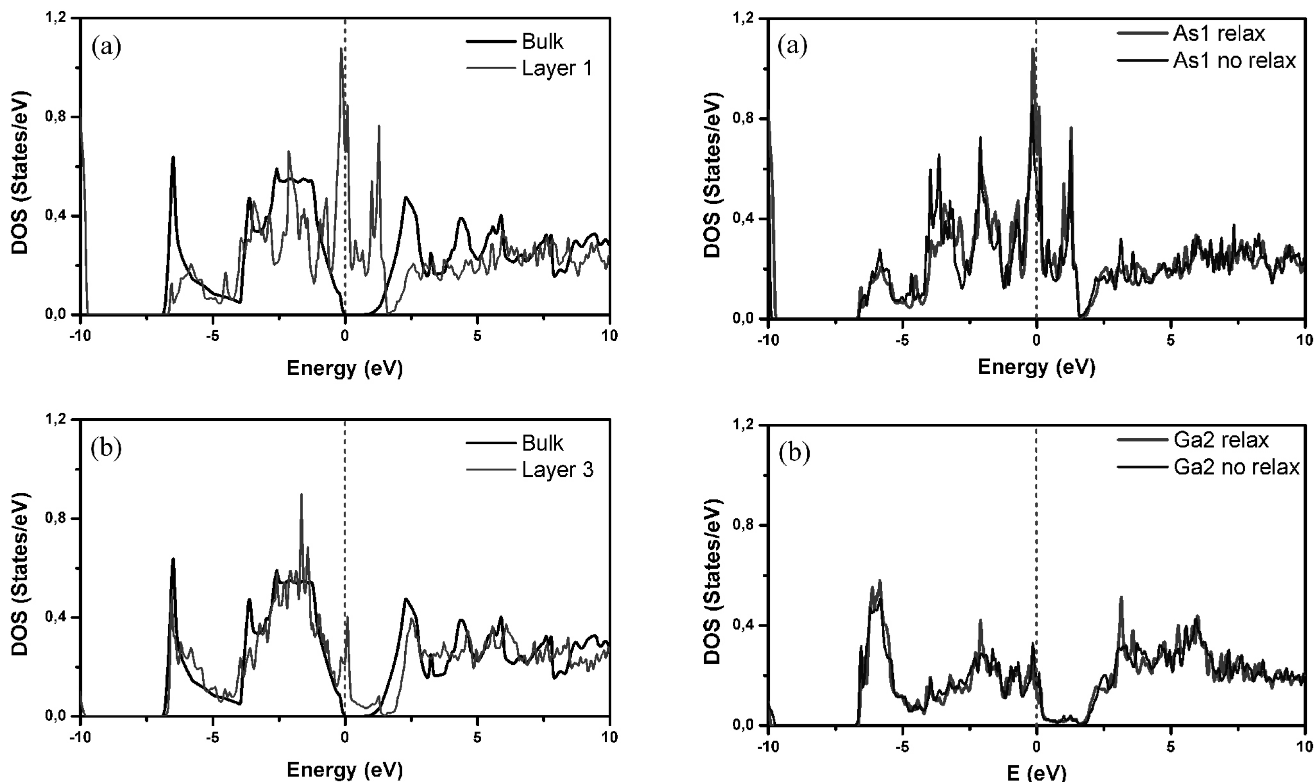

FIGURE 4. (Color online) Here we compare the As-atomic layer LDOS when in bulk and at the interface. In (a) right at the interface and (b) on the third layer from the interface.

have used the option included in the Wien2k code for that purpose. We concentrated on the $YBa_2Cu_3O_7$/GaAs interface and compared the density of states projected on two atomic layers (As and Ge) on the semiconductor side and also on the first atomic layer (CuO) on the YBCO7 side. We present our results in Fig. 5.

As we can see, relaxation has a minor effect on the density of states although some changes occur, namely, the semiconductor/superconductor distance changes from 1.49 Å (no relaxation) to 1.66 Å. This is close to 1.47 Å which is the distance between the atomic layers in the semiconductor. So relaxation does manifest itself in the crystal structure of the interface but the conclusion that four atomic layers in the semiconductor side of the interface become mettallic prevails. We did not consider other interfaces for relaxation since it is clear from the example just studied that the general result of this work, namely, that some atomic layers in the semiconductor side of the interface become mettallic, will not be altered in any essential way.

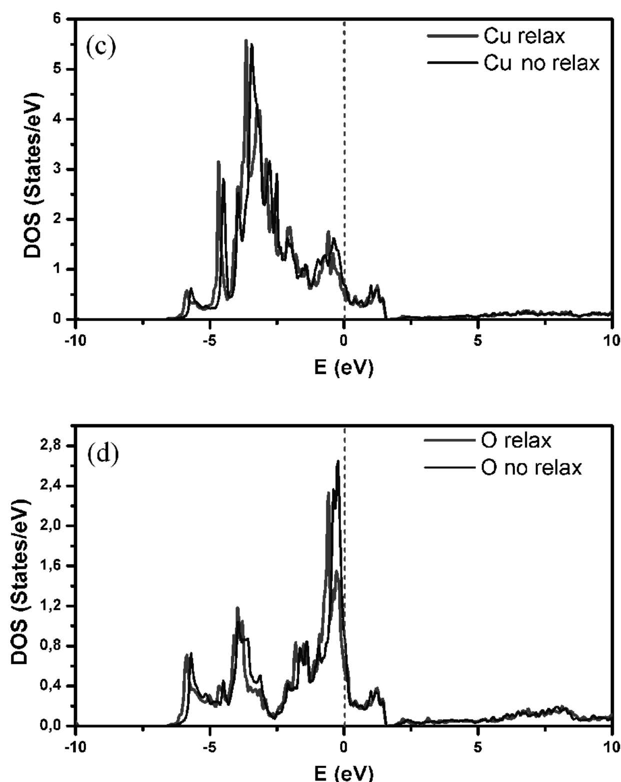

FIGURE 5. (Color online) We compare in this figure the relaxed to the non-relaxed DOS projected on the first atomic kayers from the interface at the semiconductor side and at the YBCO7 side. (a) First atomic layer (As) at the semiconductor side (b) Second atomic layer (Ga). (c) On the first atomic layer on the YBCO7 side: Contribution to the DOS from Cu, (d) from O.

6. Conclusion

In this work, we have considered twelve ideal non-reconstructed interfaces (001)YBCO7/GaZ with Z=Al, As and we find that in all the interfaces considered, the first four planes on the semiconductor side are metallic, this behaviour attenuates slowly and it tends to behave back as a semicon-

semiconductor. This effect is interesting *per se* and it can be also useful for technological applications. In these interfaces, whether the first element interacting with the metal is of the IIIA or the VA group, plays a role and does make a noticeable difference in the detailed character of the band structure at the semiconductor side. On the contrary, whether the gap of the semiconductor is direct or indirect has a much less influence or almost none at all. On the other hand, the more active layers in YBCO7 side are respectively CuO_2, BaO and CuO regardless of the plane right at the interface. We further studied the effect of relaxation on the YBCO7-GaAs interface and found that, in spite of the fact that some atomic layers change their respective distance, the influence on the density of states projected on the atomic layers on the semiconductor side change but very little as can be observed in Fig. 5. The important conslusion that four atomic layers in the semiconductor side of the interface change their character to metallic, prevails.

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