Metallic behavior at YBaCuO7/ZAs interfaces (Z=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 in the semiconductor side. The two first atomic layers in the semiconductor side of the interface present a clear metallic behavior. We found for both semiconductors considered that it converges towards the bulk atomic-layer projected density of states at the fifth atomic layer from the interface. We considered an ideal non-reconstructed interface in the (001) direction in this work. This behavior is interesting and could be used in several technological applications.

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I. INTRODUCTION

$YBa_2Cu_3O_7$ is a second generation superconductor with a $T_c$ of the order of $90K$\(^1\), Its potential applications include electric hybrid circuits\(^2\), hybrid transistors superconductor-semiconductor\(^3\), magnetic microinterruptors\(^4\), light-emitting diodes\(^5\) and diode-detectors\(^6\), among others\(^7,8\). The possible change of character at the semiconductor side of a superconductor/semiconductor interface, could allow the semiconductor well establish technology to take advantage of the known properties of superconductors for technological applications.

Interfaces containing YBCO7 have been studied experimentally\(^9\) as well as theoretically\(^10\) since long ago. Nevertheless, the semiconductor/ superconductor interfaces have been scarcely studied except for some oxides\(^11\).

In general, the change of character at an interface is of interest. A metallic behavior, for example, has been obtained at a semiconductor/semiconductor interface\(^12\), 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 advantages 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\(^13,14\), for example. Also, interfaces with semiconductors as one of the components are of interest in spintronics and spin polarized transport\(^15\).

II. COMPUTATIONAL DETAILS

We use in our calculations the Density Functional Theory (DFT)\(^16,17\) with Linearized Augmented Planes Waves plus local orbitals (LAPW+lo)\(^18\) as implemented in the Wien2k code\(^19\) 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 $R_{mt}K_{\text{max}} = 7.0$ The Muffin-tin radius, $R_{mt}$ was 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 show in Fig. 1a. When in the configuration 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 for 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 YBa2Cu3O7 (spatial group Pmmm), with lattice parameters $a = 3.8231$, $b = 3.8864$, $c = 11.6807$ 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 ($l_{GaAs} = 5.6583\AA$, $l_{AlAs} = 5.6611\AA$) and were calculated in the following way. The $x$ and $y$ axis parameters (parallel to the $a$ and $b$ axis of the superconductor) are given by

$$l_{j\parallel} = \sqrt{a^2 + \sigma_{ST} f_j b^2}$$

In the $z$-direction, the semiconductor lattice parameter is given by\(^20\)

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

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where
\[
\Delta l_j = l_j - l_{j\parallel} = -f_j.
\]  
(3)

The \(\sigma_{ST}^j\) parameter is
\[
\sigma_{ST}^j = \frac{C_{11}^j}{2C_{12}^j}
\]  
(4)

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

### III. 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, \(X=\text{AsGa}\) (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 adjacent 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 chainO/X, where \(X\) has the same definition as before (See Fig. 1b). We took the distance at the interfaces as \(d = 2.0\ \text{Å}\) so that all core states lie inside the muffin-tin sphere.

3. The third series of calculations were performed with CuO2-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 \(d = 2.2\ \text{Å}\) so that all core states lie inside the muffin-tin sphere.

### IV. 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 of 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 interface chain/GaAs. 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. 2c, we present the first two atomic layers of the interface chain/AlAs. Here again we can see that the two atomic layers are metallic.
In general, our results show that all the interfaces of the form chain/AsZ, chain/O/AsZ and plane/AsZ behave as 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 loses charge the most, as it is evident from Fig. 3c. Looking in more detail, oxygen in both, the CuO and the CuO$_2$ planes loses about the same amount of charge. The Cu atoms at these planes lose the most while the Ba atoms and the BaO planes lose 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.
V. CONCLUSION

In this work, we have considered twelve ideal non-reconstructed interfaces (001)\(Y\)\(BCO_7/GaZ\) with \(Z = \text{Al, As}\) and calculated the Local Density of States (LDOS). The interfaces considered, \(\text{chain/GaX, chain}_O/GaX\) and \(\text{plane/GaX}\), where \(\text{chain}\) (\(\text{plane}\)) refers to interfaces where the contact with the semiconductor is with the chain \(\text{CuO}_2\) plane of \(Y\)\(BCO_7\). The \(X\) stands for \(\text{Al or As}\). The order in which they appear in this work, as \(\text{plane/AsGa}\), for example, means that the interface begins with an atomic plane of \(\text{As atoms}\) at the semiconductor side. We distinguish between \(\text{chain/GaX}\) and \(\text{chain}_O/GaX\), meaning that in the last case, the \(\text{Ga}\) atoms face the oxygens of the \(\text{CuO}\) chains. The main conclusion is that all the interfaces considered present several planes on the semiconductor side that are metallic. This behavior attenuates slowly and end at the fifth layer where the material behaves back as a semiconductor. This effect is interesting \textit{per se} and it can be also useful for certain technological applications.

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1M. K. Wu, J. R. Ashburn, C. J. Torng, P. H. Hor, R. L. Meng, L. Gao, Z. J. Huang, Y. Q. Wang, and C. W. Chu, Phys. Rev. Lett. \textbf{58}, 908 (1987)
2K. B. Bhasin, S.S. Tonchich, C.M. Chorey, R.R. Bonetii, A.E. Williams, IEEE MTT-S Dig. \textbf{1}, 481 (1992)
3D. J. Frank, Cryogenics \textbf{30}, 996 (1990)
4C. Castellana, F. Giazotto, M. Governale, F. Taddei, and F. Beltram, Appl. Phys. Lett. \textbf{88}, 052502 (2006)
5H. Sasakura, S. Kuramitsu, Y. Hayashi, K. Tanaka, T. Akazaki, E. Hanamura, R. Inoue, H. Takayanagi, Y. Asano, C. Hermannsdter, H. Kumano, and I. Suemune, Phys. Rev. Lett. \textbf{107}, 157403 (2011)
6M. McColl, M. F. Millea, and A. H. Silver, Appl. Phys. Lett. \textbf{23}, 263 (1973)
7U. Ghoshal, H. Kroger and T. Van Duzer, IEEE Trans. Appl. Supercond. \textbf{3}, 2315 (1993)
8U. Ghoshal, H. Kroger, US Patent 5388068, 1995.
9B.D. Hunt, M.C. Foote and L. Bajuk, IEEE Trans. Magn. \textbf{27}, 848 (1991)
10U. Schwingenschlgl and C. Shuster, Appl. Phys. Lett. \textbf{90}, 192502 (2007)
11K. Sakuta, M. Iyori, T. Kobayashi, M. Matsui and M. Nakajima, IEEE Trans. Magn. \textbf{27}, 1361 (1991)
12S. Nazir and U. Schwingenschlgl, Appl. Phys. Lett. \textbf{99}, 073102 (2011)
13M. L. Cohen, Phys. Rev. \textbf{134}, A511 (1964).
14M. L. Cohen, Rev. Mod. Phys. \textbf{36}, 240 (1964).
15S. Das Sarma, J. Fabian, X. Hu, and I. Zutic, IEEE Trans. Magn. \textbf{36}, 2821 (2000).
16P. Hohenberg and W. Kohn, Phys. Rev. \textbf{136}, B864 (1964).
17W. Kohn and L. J. Sham, Phys. Rev. \textbf{140}, A1133 (1965).
18G. K. H. Madsen, P. Blaha, K. Schwarz, E. Sjsttedt, and L. Nordstrm, Phys. Rev. B \textbf{64}, 195134 (2001).
19P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2k, An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties (Vienna University of Technology, Austria, 2001).
20P. Bhattacharyya, Semiconductor Optoelectronic Devices, 2nd ed. (Prentice-Hall, Upper Saddle River, NJ, 1997), p. 22.
21M. A. Beno, L. Soderholm, D. W. Capone, D. G. Hinks, J. D. Jorgensen, J. D. Grace, I. K. Schuller, C. U. Segre, and K. Zhang, Appl. Phys. Lett. \textbf{51}, 57 (1987)
22I. E. Ayers, Heteroepitaxy of Semiconductors: Theory, Growth, and Characterization (CRC, Boca Raton, 2007), p. 208.