Geometry dependence of the charge transfer at YBa$_2$Cu$_3$O$_7$-metal interfaces

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Transport in electronic devices based on high-T_c superconductors depends critically on the charge redistribution at interfaces, since the band structure is modified on a local scale. Using the density functional theory approach for relaxed YBa$_2$Cu$_3$O$_7$-metal contacts, the charge transfer into the superconductor has been studied [U. Schwingenschlögl and C. Schuster, Appl. Phys. Lett. **90**, 192502 (2007)]. In the present paper we discuss the systematics inherent in the local electronic structure of the near-contact YBa$_2$Cu$_3$O$_7$ sites, in particular, the dependence on the contact geometry. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2821363]

I. INTRODUCTION

Due to large dielectric constants and small carrier[1] densities, electronic transport in wires and tapes from high-T_c materials is seriously affected by structural defects and interfaces.[2,3] Moreover, the specific contact resistivity of YBa$_2$Cu$_3$O$_7$ (YBCO)-metal thin films is determined by details of the contact geometry,[4] and the transport in micrometer-sized YBCO-metal heterojunctions depends on the orientation of the YBCO crystallographic axes with respect to the direction of the current flow.[5] Unexpected high specific resistivities of YBCO-Au interfaces, 10^{-4} Ω cm^2 to 10^{-3} Ω cm^2 at low temperatures,[6] presumably result from local distortions at the interface. While theoretical attempts to describe the charge distribution at such interfaces are rare, the linear background and asymmetry in the differential conductance of a tunnel junction between a high-T_c superconductor and a metal can be explained by inelastic scattering.[7] In addition, the charge imbalance at the boundary of a short-coherence-length superconductor and a normal metal is accessible to a self-consistent microscopic approach.[8]

II. TECHNICAL DETAILS

Taking into account the details of the crystal structure, the electronic properties of YBCO-metal interfaces can be addressed by means of first-principles band structure calculations.[9] In this paper we investigate the dependence of the local electronic structure in the YBCO domain on the contact geometry. As YBa$_2$Cu$_3$O$_7$ belongs to the overdoped regime, our interfaces are metallic. The calculations are based on density functional theory and the generalized gradient approximation, as implemented in the WIEN2K program package,[10] which is suitable for dealing with structural relaxation and charge redistribution at surfaces and interfaces.[11,12] Because band-bending is proposed to take place on the length scale of the YBCO lattice constant, the electronic structure of YBCO-metal interfaces becomes accessible to a supercell approach with periodic boundary conditions. Due

to a minimal lattice mismatch of $\approx$0.7%, it is convenient to choose fcc Pd as metallic substituent.

We study interfaces oriented parallel and perpendicular to the CuO$_2$ planes. The parallel interface is modelled by means of a supercell consisting of two YBCO unit cells along the crystallographical c-axis, terminated by the CuO-chain layer,[13,14] and four metallic unit cells stacked in [001] direction. However, the results are closely related to those for BaO-terminated YBCO. The perpendicular interface consists of three YBCO unit cells and a 3×3 metallic supercell stacked in [010] direction. In total, the supercell therefore contains nine metallic unit cells. We again chose a CuO/Pd interface to prepare for comparison with the parallel configuration. In contrast to the latter, oxygen atoms from the BaO planes and copper atoms from the CuO$_2$ planes here likewise touch the metal layer. Giving rise to the main difference between the two configurations, in the parallel configuration the CuO$_2$ planes are well separated from the metal by an almost insulating BaO layer, whereas they are in contact in the perpendicular configuration. The Y atoms are in touch with the metal layer only in the latter case. Relative shifts between the YBCO and metal domain parallel to the interface have minor effects. We start from the experimental bulk YBCO lattice constants $a=3.865$ Å and $b=3.879$ Å,[15] and optimize the atomic coordinates in a first step.[16] Parallel to the interface, the YBCO lattice constants are used for the palladium domain, too. In the perpendicular direction, we apply the fcc Pd lattice constant $c=3.89$ Å. In a second step, the structural relaxation of the supercells is carried out, see Ref. 17 for details of the structure optimization.

III. RESULTS

In the following discussion, we compare the electronic structures of our YBCO-metal interfaces with results of a bulk YBCO calculation (which agree perfectly with previous findings[18]). In addition, we will concentrate on atomic sites slightly off the YBCO-metal contact in order to determine a common behavior. These sites are less affected by the structural optimization, whereas the electronic properties of atoms right at the interface depend strongly on structural subtleties and therefore are not of interest here. We first study the par-

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FIG. 1. (Color online) Partial Ba and Y DOS.

FIG. 2. (Color online) Partial Cu 3*d* DOS for the CuO$_2$ planes and CuO chains.
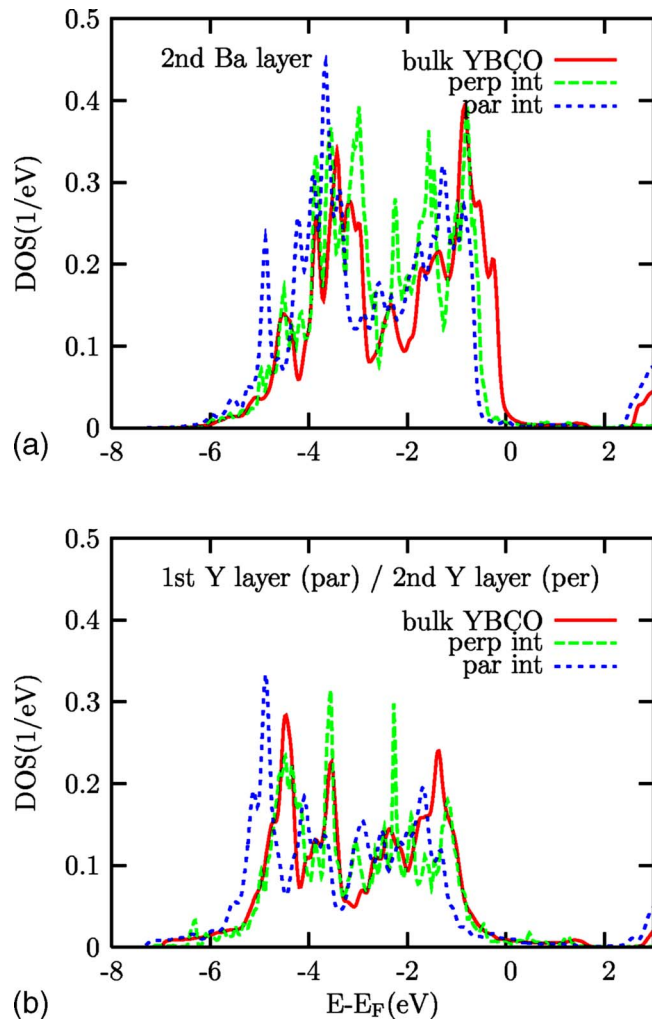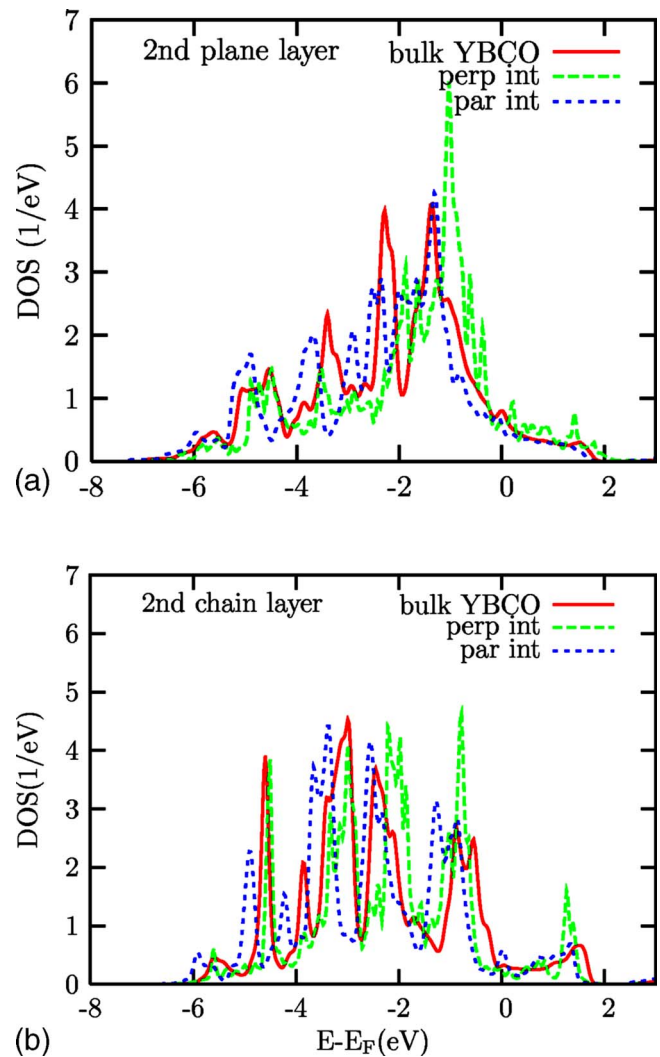
tial density of states (DOS) associated with the Ba and Y electron donor sites (see the DOS curves in Fig. 1). For both geometries, the second Ba layer off the interface is well separated from the metal domain. As a consequence, the gross features of the DOS curves agree well with each other as well as with the bulk YBCO DOS, when an adequate energetical shift of about −0.45 eV is applied. In contrast, the Y DOS curves hardly coincide, which traces back to large differences in the local atomic environments of the Y sites in the parallel and perpendicular interface configuration. The first Y layer off the parallel interface is well separated from the metal by four atomic layers. The energetical shift of the Y states therefore can be attributed to strong down-bending of the electronic bands due to a modified Fermi level. At the perpendicular interface, Y–Pd orbital overlap suppresses band-bending effects. While the Y DOS reveals a finite number of states at the Fermi level, the Ba DOS almost vanishes. Electronic screening thus is less efficient at the Ba sites and the band-bending amplitude increases.

Turning to the copper sites, the gross structure of the Cu 3*d* DOS is hardly affected by the interface (see Fig. 2). The second-layer Cu atoms largely resemble the bulk DOS and therefore allow us to study the band-bending. Concerning the CuO-chain sites, results for the parallel and perpen-

dicular interface configuration agree quite well. Similar to the discussion of the Y DOS, the smaller energy shift in the perpendicular case can be explained by direct Cu–Pd orbital overlap. Understanding the DOS shape of the CuO$_2$-plane sites is less intuitive. For the parallel interface, we observe almost perfect agreement of the DOS curves, whereas some effects of the structural relaxation are left for the perpendicular interface. However, in both cases the bulk DOS has to be shifted to lower energies in order to reconcile the curves, which we again interpret in terms of down-bending of the electronic bands. The necessary shifts amount to 0.20 eV and 0.15 eV in the parallel and perpendicular case, respectively. As a consequence, the hole count at the Cu sites in the CuO$_2$ planes is altered, where the 0.20 eV shift corresponds to a reduction of 0.13 holes, and the 0.15 eV shift comes along with a reduction of 0.09 holes. Since the charge transfer depends only little on the orientation of the YBCO-metal interface with respect to the high-T_c unit cell, an intrinsic doping close to 0.1 eV seems to be characteristic for YBCO-metal contacts. As a consequence, the system is shifted into the underdoped regime of the YBCO phase diagram, which is expected to be reflected by transport properties, like the current in tunneling experiments.

IV. CONCLUSION

In conclusion, we have discussed electronic structure calculations for prototypical interfaces between the short-coherence-length superconductor $YBa_2Cu_3O_7$ and a normal metal. We find that the charge redistribution induced by the metal contact can be interpreted in terms of an intrinsic doping of the superconductor on a nanometer length scale. This fact corresponds well with the experimental observation of charge carrier depletion. The net charge transfer in favor of the copper sites in the CuO_2 planes amounts to some 0.1 electrons, with only a weak dependence on the orientation of the interface. We expect that the reported charge-transfer amplitude applies to any contact geometry as long as the YBCO domain terminates with a copper/oxygen layer.

ACKNOWLEDGMENTS

[1]G. A. Samara, W. F. Hammetter, and E. L. Venturini, Phys. Rev. B **41**, 8974 (1990).
[2]J. Mannhart and H. Hilgenkamp, Mater. Sci. Eng., B **56**, 77 (1998).
[3]H. Hilgenkamp and J. Mannhart, Rev. Mod. Phys. **74**, 485 (2002).
[4]R. Hahn, J. Klockau, and G. Fotheringham, Supercond. Sci. Technol. **7**, 290 (1994).
[5]F. V. Komissinskii, G. A. Ovsyannikov, and Z. G. Ivanov, Phys. Solid State **43**, 801 (2001).
[6]Y. Xu and J. W. Ekin, Phys. Rev. B **69**, 104515 (2004).
[7]M. Grajcar, A. Plecenik, P. Seidel, V. Vojtanik, and K. U. Barholz, Phys. Rev. B **55**, 11738 (1997).
[8]B. K. Nikolić, J. K. Freericks, and P. Miller, Phys. Rev. B **65**, 064529 (2002).
[9]U. Schwingenschlögl and C. Schuster, Appl. Phys. Lett. **90**, 192502 (2007).
[10]P. Blaha, K. Schwarz, G. Madsen, D. Kvasicka, and J. Luitz, WIEN2K, An augmented plane wave + local orbitals program for calculating crystal properties (TU Wien, 2001).
[11]U. Schwingenschlögl and C. Schuster, Chem. Phys. Lett. **435**, 100 (2007); **439**, 143 (2007).
[12]U. Schwingenschlögl and C. Schuster, Chem. Phys. Lett. **449**, 125 (2007); Europhys. Lett. **81**, 17007 (2008); **81**, 26001 (2008).
[13]G. Xin-Gao and Z. Qing-Qi, J. Phys.: Condens. Matter. **1**, 593 (1989).
[14]D. J. Derro, E. W. Hudson, K. M. Lang, S. H. Pan, J. C. Davis, J. T. Markert, and A. L. de Lozanne, Phys. Rev. Lett. **88**, 097002 (2002).
[15]T. Siegrist, S. Sunshine, D. W. Murphy, R. J. Cava, and S. M. Zahurak, Phys. Rev. B **35**, 7137 (1987).
[16]R. Kouba, C. Ambrosch-Draxl, and B. Zangger, Phys. Rev. B **60**, 9321 (1999).
[17]U. Schwingenschlögl and C. Schuster, Europhys. Lett. **77**, 37007 (2007).
[18]W. E. Pickett, Rev. Mod. Phys. **61**, 433 (1989).