Anomalous surface overdoping as a clue to the puzzling electronic structure of YBCO-123

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Available online 2 April 2007

Abstract

We show that the photoelectron spectrum of YBCO-123 generally includes two components. The one, which is the most pronounced, is characterized by unusually high hole doping level and exhibits no superconducting gap, while the other component retains superconductivity. We believe, the occurrence of these two components in ARPES spectra was one of the reasons that caused difficulties with the interpretation of earlier ARPES data of this compound.
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According to tight binding calculations, the bilayer splitting and the quasi-one-dimensional bands arising due to Cu–O chains have to be the most prominent features in the low-energy electronic structure of YBCO-123. While in one of the earliest works [1] two features forming an extended saddle point along the Γ–X/Y direction at energies of about 19 and 150 meV were believed to be the bonding and the antibonding bands, in the Refs. [2,3] the low-energy feature (19 meV) was identified as a surface state, while the bonding and the antibonding bands were believed to lie at significantly higher binding energies. In one of the most recent works [4], done with improved instrumental resolution, the feature with the highest binding energy was ascribed to the chain states, and, contrary to the two previous investigations, no clear evidence of bilayer splitting was reported. In addition, unusually small or vanishing gaps observed in many ARPES investigations

of YBCO [1,5,6] make the interpretation of the ARPES spectra for this compound even more perplexing. Therefore, to bring all these data under one common description, further experimental work is required.

The spectra discussed here were measured at the U125/1-PGM beam line (BESSY) using a SCIENTA SES100 spectrometer from freshly cleaved surfaces at $T = 30$ K. The energy resolution was set to 15 meV for measurements done with 50 eV excitation energy and to 25 meV, for the spectra measured with $hv = 100$ eV. The angular resolution was 0.2°. The high quality YBCO samples were prepared by the solution-growth method, annealed to achieve the desired oxygen content, and detwinned by mechanical pressure [7].

In Fig. 1a we show a typical Fermi surface (FS) for the nearly optimally doped YBCO-123. Owing to the high quality of the crystals and appropriate choice of the excitation energy, the features are well pronounced and sharp, so that bilayer split bands can be unambiguously identified without resorting to any complicated data treatment like

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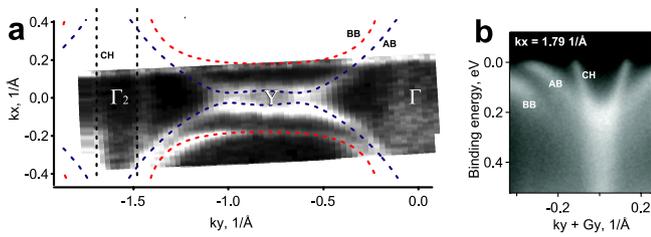* Corresponding author.
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Fig. 1. (a) FS of $YBa_2Cu_3O_{7-\delta}$ ($T_c \sim 90$ K) and TB fit. (b) Momentum energy intensity distribution with all low-energy features well resolved: CH – chain band; AB – antibonding band; BB – bonding band. $G_y \approx 1.64$ Å^{-1} is a component of the reciprocal lattice vector.

Fig. 2. Energy-momentum maps for $YBa_2Cu_3O_{6.6}$, ($T_c = 61$ K, $hv = 50$ eV).

taking the 2nd derivative. It is also easy to recognize that the two weaker features, parallel to the k_x axis, correspond to a quasi-one-dimensional chain band. Following the predictions of the LDA calculations [8], the dispersion of all the bands can easily be traced from the Fermi level (FL) down to binding energies of about 200 meV, as it can be seen from energy-momentum intensity distribution given in Fig. 1b.

Although measuring at temperatures much below T_c, neither analysis of the leading edge gap positions nor the experimental band dispersion support the existence of a superconducting gap larger than 10 meV, as one would expect to observe for the optimally doped sample. Using the advantage of having the full FS, we made a tight binding fit to the bonding and antibonding band FL crossings and found the hole doping level to be about 0.30. Similar overdoping of the near-surface region was observed in our numerous subsequent measurements for samples with the same stoichiometry, proving this to be a robust effect. We believe that this overdoping effect provides a natural explanation for the problems experienced with gap observation in ARPES and STM experiments and also dispels an apparent contradiction between the high $T_c \sim 90$ K of the sample and the doping level of the crystal near-surface region that is modified after cleavage.

The ARPES technique can also provide us with information about the thickness of the overdoped near-surface region. A closer look at the EDCs in the vicinity of the X/Y point, in addition to the two peaks from overdoped bilayer split bands, always reveals the presence of an extra peak (not shown here) at energies about 40–50 meV that practically disappears above T_c, similar to the one observed in [4]. By tuning the polarization and the excitation energy it was possible to partly suppress the photoemission from the overdoped component, so that the whole spectrum attained familiar superconducting features, like those normally observed in the Bi-2212 system [9,10]. In Fig. 2a
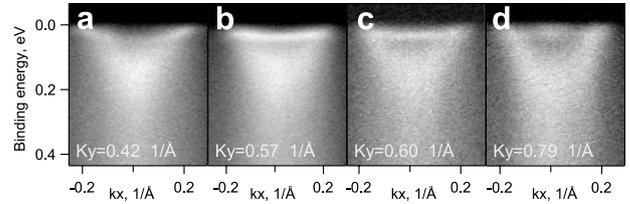
we can see the widely discussed kinks in the band dispersion at the energy of about 50 meV. When moving closer to the Y point (panel b), similar to Bi-2212, the renormalization becomes so strong that the spectral weight gets concentrated in one practically flat and non-dispersing feature. However, at the very vicinity of the Y point the overdoped component takes over again. In panel (d) one can notice the appearance of the antibonding band of the overdoped component as well as the increase of the spectral weight at the FL, which becomes especially pronounced when comparing to image (b). The fact that it is possible to detect the superconducting component in the ARPES experiment tells us that the thickness of the overdoped layer is of the order of the photoelectron penetration depth, i.e., 5–10 Å and is comparable to one lattice spacing along the c-axis.

To conclude, we have shown that the low-energy electronic structure of YBCO-123 is generally consistent with LDA calculations and that the "non-superconducting" character of ARPES spectra may result from strong overdoping of the prepared by cleaving surface.

Acknowledgements

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