Doping Evolution of a Superconducting-Gap Anisotropy in $YBa_2Cu_3O_{7-\delta}$ Studied by High-Resolution Angle-Resolved Photoemission Spectroscopy

We have performed high-resolution angle-resolved photoemission spectroscopy of the high-temperature (T_c) superconductor $YBa_2Cu_3O_{7-\delta}$ with various hole concentrations ranging from under- to optimal-doping. By extracting the bulk electronic states with circularly polarized photons of synchrotron radiation, we have accurately determined the momentum dependence of the superconducting gap as a function of hole concentration. The observed enhancement of the maximal gap size and the deviation from a simple $d_{x^2-y^2}$-wave symmetry in the underdoped region suggest that the pairing interactions become stronger and act over a longer range for under-doping. The present results provide evidence for similar character of the low-energy excitation gap in bilayered copper oxide high-T_c superconductors.

Investigation of the superconducting (SC) gap function is essentially important for elucidating the SC mechanism, since its anisotropy in momentum space and its magnitude are intimately related to the pairing interactions and the pairing strength, respectively. In copper oxide high-T_c superconductors, while the opening of a $d_{x^2-y^2}$-wave SC gap has been observed in $Bi_2Sr_2CaCu_2O_8$ (Bi2212) [1], a possible T_c or crystal structure dependence of the SC-gap function has been recently reported [2, 3]. In this regard, $YBa_2Cu_3O_{7-\delta}$ (YBCO) is an ideal candidate for study, since its crystal structure is different from that of Bi2212. While YBCO is a bilayered system with a maximum T_c value comparable to that of Bi2212, there is a marked difference in the T_c vs doping relation between Bi2212 and YBCO [4]. It is thus particularly important to elucidate the bulk SC-gap character of YBCO. However, angle-resolved photoemission spectroscopy (ARPES) studies of the bulk electronic states of YBCO have been difficult due to the presence of surface states [5].

We have performed high-resolution ARPES measurements at BL-28A with untwinned YBCO single crystals for three different doping levels. The samples used were under-doped samples with T_c = 60 K and 80 K, and a near-optimally doped sample with T_c = 92 K, hereafter referred to as UD60K, UD80K and OP92K, respectively [6].

Figures 1(a)-(c) show plots of the ARPES intensity at E_F as a function of the two-dimensional wave vector for (a) UD60K, (b) UD80K and (c) OP92K YBCO. We find two large Fermi surfaces (FSs) centered at the S point in the Brillouin zone. The hole concentrations (p) estimated from the FS volumes are 0.27±0.02, 0.29±0.02 and 0.29±0.02 holes/Cu for the UD60K, UD80K and OP92K samples, respectively. The invariance of p suggests that the observed FSs do not reflect the bulk properties, and can be attributed to surface states derived from the cleaved topmost CuO_2 bilayer [7]. As seen in Figs. 1(d)-(f), the metallic surface bands, denoted by gray circles, show asymmetric intensity variations with respect to the ΓY high-symmetry line, consistent with the expected circular dichroism for the surface states [8]. In the momentum location where the spectral intensity of the surface bands is significantly suppressed (the area enclosed by a white circle), we can identify additional bands with energy dispersions different from that of the surface bands. We assign these bands to the bulk bands, since they show characteristic features of bulk CuO_2 planes similar to Bi2212 (*e.g.* a SC gap opening and a strong mass renormalization below T_c) [6, 7].

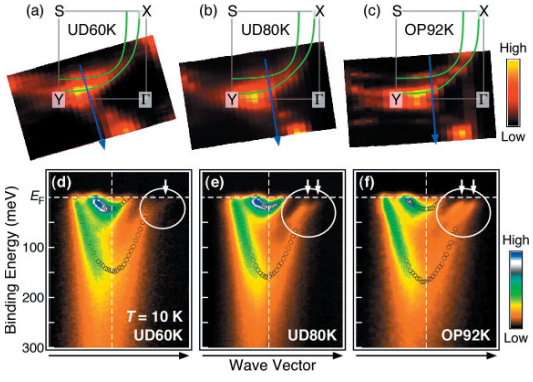

Figure 1
ARPES intensity plots at E_F as a function of the two-dimensional wave vector measured at 10 K for (a) UD60K, (b) UD80K and (c) OP92K YBCO. The green curves are the experimentally determined FSs of the surface bands. (d)-(e) ARPES intensity plots as a function of binding energy and wave vector measured along the blue arrows shown in (a)-(c). The gray circles show the surface-band dispersions determined from the peak positions in the ARPES spectra after eliminating the effects of the Fermi-Dirac distribution function. The white arrows represent the positions of the k_F points for the bulk bands.

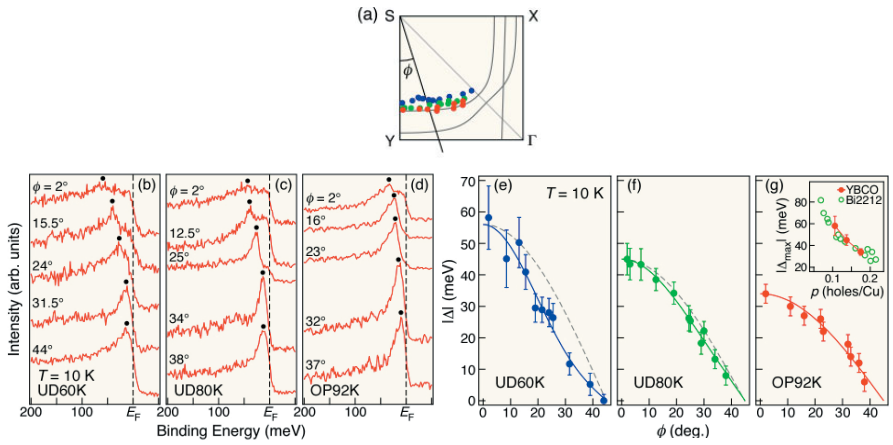

Figure 2
(a) Locations of the k_F points of the bulk bands for UD60K (blue dots), UD80K (green dots) and OP92K (red dots) samples of YBCO together with the definition of the FS angle (ϕ). (b)-(d) ARPES spectra after background subtraction at 10 K measured at various k_F points of the bulk bands for the (b) UD60K, (c) UD80K and (d) OP92K samples. The black dots denote the peak positions corresponding to the bulk bands. Momentum (FS angle, ϕ) dependence of SC gap size at 10 K for (e) UD60K, (f) UD80 and (g) OP92K samples. The dashed lines show the energy gaps for an ideal $d_{x^2-y^2}$-wave symmetry. The solid curves show the best fit results to the gap function $|\Delta|=|\Delta_{max}|\{B\cos2\phi+(1-B)\cos6\phi)\}$ [10]. The inset to (g) shows the doping dependence of $|\Delta_{max}|$ determined in the current study (red dots) compared with the previous ARPES experiments on Bi2212 ([9], green circles).

To clarify the doping dependence of the SC-gap symmetry, we determined the k_F points of the bulk bands. As can be seen in Fig. 2(a), the FS volume monotonically decreases with under-doping, indicative of the bulk nature of these bands. Figures 2(b)-(d) show ARPES spectra measured at 10 K at various k_F points of the bulk band. In all the doping levels, the energy position of the bulk SC peak, which basically corresponds to the SC-gap size (Δ), is strongly k dependent and gradually becomes smaller approaching the nodal direction (ϕ=45°), showing an overall $d_{x^2-y^2}$-like gap symmetry. The Fermi-edge structure in the antinodal region (ϕ~0°), which originates from the surface band, does not affect the estimation of SC-gap size, since it is well separated from the bulk SC peak. It is apparent from Figs. 2(e)-(g) that the maximal SC-gap size systematically increases with less doping, suggesting stronger pairing interactions in the under-doped region. This behavior is quantitatively consistent with previous ARPES results of Bi2212 [9] as shown in the inset to (g). It is also remarked that while the gap anisotropy in the OP92K sample is well characterized by the simple $d_{x^2-y^2}$-wave formula ($|\Delta|=|\Delta_{max}|\cos2\phi$), we find a finite deviation in the under-doped region. The observed gap anisotropy in the under-doped region can be well reproduced by taking into account the higher harmonic term of the $d_{x^2-y^2}$-wave $[|\Delta|=|\Delta_{max}|\{B\cos2\phi+(1-B)\cos6\phi)\}]$ [10], as can be clearly seen in Figs. 2(e)-(g). This suggests the importance of long-range interactions for the SC pairing [10] in under-doped YBCO. The obtained fitting parameter B is 0.85, 0.95 and 1.0 for the UD60K, UD80K and OP92K samples, respectively. This variation shows a quantitatively good agreement with the results for Bi2212 [10]. These experimental results provide evidence for the similarity of the low-energy excitation gaps of YBCO and Bi2212.

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