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Physical Review B
Volume 67
Number 6
Page range 060501
Year 2003-02

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URL http://hdl.handle.net/2241/89246
doi: 10.1103/PhysRevB.67.060501
Systematics of electronic structure and interactions in Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n=1-3$) by angle-resolved photoemission spectroscopy


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Received 19 November 2002; published 28 February 2003

We have performed systematic angle-resolved photoemission spectroscopy on the high-$T_c$ superconducting family of Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n=1-3$). In addition to the generic features of the large Fermi surface and $d$-wave superconducting gap, we have found that there exists a scaling of the doping dependence of the energy gap. Moreover, comparison of the nodal dispersion in the superconducting state shows that the “kink” (the sudden change of band dispersion), while occurring at a similar binding energy, becomes more pronounced with increasing layer number $n$, indicating stronger coupling between electrons and a collective mode.

DOI: 10.1103/PhysRevB.67.060501

PACS number(s): 74.72.Hs, 71.18.+y, 74.25.Jh, 79.60.Bm

It has been well established that the CuO$_2$ plane is a key block in the crystal structure to realize the high-temperature (high-$T_c$) superconductivity in cuprates. It is empirically known that the superconducting-transition temperature ($T_c$) increases with an increasing number of CuO$_2$ planes ($n$) in a unit cell of the crystal. For example, in Bi-family high-$T_c$ superconductors (HTSCs), $T_c$ increases from 10 K for single-layered Bi$_2$Sr$_2$CuO$_4$ (Bi2201) to 90 K for bilayered Bi$_2$Sr$_2$CaCu$_2$O$_8$ (Bi2212), and further to 110 K for trilayered Bi$_2$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ (Bi2223). This suggests that the interlayer interaction is important to achieve higher $T_c$, and that the variation of $T_c$ with $n$ may be a certain universal rule relating to $n$. However, despite intensive theoretical and experimental studies, the microscopic origin to enhance $T_c$ in multilayered cuprates is still unknown. It is thus urgently required to clarify differences and similarities in the electronic structure, in particular in the low-energy excitation which directly relates to the superconductivity, among single- to multilayered high-$T_c$ cuprates.

Angle-resolved photoemission spectroscopy (ARPES) has revealed the essential electronic structure of high-$T_c$ cuprates such as Fermi surface and superconducting gap. Recent improvement in the energy resolution in ARPES has enabled direct observation of low-energy excitation as well as the interaction between two CuO$_2$ planes (bilayer band splitting). However, in contrast to intensive ARPES studies on bilayered cuprates (Bi2212), few ARPES works to systematically study the electronic structure near the Fermi level ($E_F$) as a function of CuO$_2$ planes have been reported. This is because of the difficulty in growing a high-quality trilayered single crystal (Bi2223). Comparison among these three Bi-family HTSCs would reveal not only the basic electronic structure irrespective of the number of CuO$_2$ planes ($n$), but also, more importantly, the difference in the low-energy excitation for different $n$ compounds, which is crucial to find key parameter(s) to enhance $T_c$ in multilayered high-$T_c$ cuprates.

In this paper, we report systematic high-resolution ARPES on Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n=1-3$) single crystals. By comparing the experimental result for $n=3$ with those for $n=1$ and 2, we discuss the universality and speciality of the basic electronic structure near $E_F$ in these three high-$T_c$ cuprates, such as the Fermi-surface (FS) topology, the superconducting-gap symmetry, and the doping dependence of the superconducting gap. We also discuss the coupling strength of electrons with collective mode(s) as a function of $n$ to study the microscopic origin to enhance $T_c$ in multilayered cuprates.

High-quality Bi$_2$Sr$_2$Ca$_{n-1}$Cu$_n$O$_{2n+4}$ ($n=1-3$) single crystals were grown by the traveling solvent floating-zone (TSFZ) method. Details of sample preparations have been described elsewhere. ARCES measurements were performed with a GAMMADATA-SCIENTA SES-200 spectrometer at the undulator 4m-NIM beamline of the Synchrotron Radiation Center, University of Wisconsin-Madison, Wisconsin, as well as with a same-type spectrometer using a high-flux discharge lamp and a toroidal grating monochromator at Tohoku University, Japan. We used 22-eV synchrotron photons and a He I resonance line (21.218 eV) to excite photoelectrons. The energy and angular (momentum) resolutions were set at 9–15 meV and 0.2° (0.007 Å$^{-1}$), respectively. Samples were cleaved in situ in an ultrahigh vacuum of $4\times10^{-11}$ Torr to obtain a clean surface for measurement. The Fermi level ($E_F$) of samples was referred to that of a gold film deposited on a metallic substrate which is in electrical contact with samples.

Figure 1 shows ARPES-intensity maps of Bi2223 as a function of the two-dimensional wave vector for an overdoped sample with $T_c=100$ K (OD100K) and an underdoped one with $T_c=108$ K (OD108K). ARPES intensity is integrated over the energy range of 50 meV centered at $E_F$. Measurements were done in the $Y$ quadrant to avoid the complication from the superlattice bands. Two intensity maxima symmetric to the $M$ point are clearly seen on $M$-$Y$($X$) line,
but not on the $\Gamma$-$M$ line. This clearly defines a large holelike FS centered at $X(Y)$ for both samples, consistent with a recent report.12 We have determined the Fermi vector ($k_F$) by fitting the momentum distribution curves (MDCs) and estimated the FS volume to be $56 \pm 2\%$ and $59 \pm 2\%$ of the whole Brillouin zone for UD100K and OD108K samples, respectively. These values correspond to $x = 0.12 \pm 0.03$ and $0.17 \pm 0.03$ where $1 + x$ is the hole count, consistent with the doping level, since the doping level at the optimally doped region is typically $x = 0.16$.13 In Figs. 1(c) and (d), we plot the ARPES intensity for Bi2212 (OPT91K: optimally doped, $T_c = 91$ K) and Bi2201 (UD19K: underdoped, $T_c = 19$ K).

One can clearly see that ARPES-intensity distributions are essentially similar to that in Bi2223, showing that the hole-like Fermi surface is a generic feature of the CuO$_2$ plane in HTSCs. It is also noted that the trilayer splitting is not clearly resolved in Bi2223, since the MDC can be fitted by a single Lorentzian. This may be due to the difference in the spectral weight distribution between Bi2223 and bilayer Bi2212, as suggested by recent theoretical14 and ARPES studies.12

Figure 2(a) shows ARPES spectra near $E_F$ for the UD100K Bi2223 sample in the superconducting state (40 K) measured on the Fermi surface ($k_F$ points) in the $Y$ quadrant [see the inset to Fig. 2(b)]. A sharp quasiparticle (QP) peak is located about 50-meV away from $E_F$ near the $M$ point (spectrum 1), and gradually moves towards $E_F$ when approaching the nodal line. No sizable leading-edge shift is observed in spectra 7–9. This momentum dependence of QP peaks clearly indicates the highly anisotropic nature of the superconducting gap in underdoped Bi2223, similar to the optimally doped Bi2223.12 In order to estimate the superconducting-gap size ($\Delta$) more accurately, we have symmetrized the spectra with respect to $E_F$ (Ref. 15) and fit each curve by two Lorentzians symmetric to $E_F$. The obtained $k$ dependence of $\Delta$ is shown in Fig. 2(b), together with those of Bi2201 and Bi2212.3,16 The overall “$V$” shape of the gap curve, as well as the node along the $\Gamma$-$Y$ line ($\phi = 45^\circ$), strongly support the $d$-wave nature of the gap in all Bi-family HTSCs. We have fit the gap size for Bi2223 as a function of $\phi$ by using the formula $\Delta(\phi) = \Delta_{\text{max}}[B\cos(2\phi) + (1-B)\cos(6\phi)]$, where the cos(6$\phi$) term represents the second harmonic of the $d_{x^2-y^2}$-gap function.17 Excellent agreement is obtained with the parameters $\Delta_{\text{max}} = 47$ meV and $B = 0.94$. A small but finite amount of the second term ($6\%$) may be due to the underdoped nature of the sample.17 It is noted here when we compare the gap size among $n = 1$–3, we find that the overall gap value systematically increases with increasing $n$, demonstrating a certain scaling of the superconducting gap.18

Next we study the doping dependence of $\Delta_{\text{max}}$. Figure 3(a) shows ARPES spectra at the superconducting state (40 K) measured at $k_F$ on the $M$-$Y$ line ($\phi = 0^\circ$) for three Bi2223 samples with different dopings (UD100K, OPT108K, and OD108K). Although the overall spectral feature such as the hump-dip-peak structure looks similar, there are quantitative differences in the spectra. When the doping is increased from UD100K to OD108K, the intensity of the QP peak is gradually enhanced and at the same time the peak position ($\Delta_{\text{max}}$) systematically moves toward $E_F$, consistent with similar behavior observed in Bi2212.3 The increase in the QP-peak intensity is consistent with the increase in the superfluid density as the hole doping is increased.19,20 In order to estimate $\Delta_{\text{max}}$ quantitatively, we have fit the ARPES spectra by a Gaussian for the QP peak and a linear function.
with an asymmetric cutoff for the hump. Both are multiplied by the Fermi-Dirac function and then convoluted by a Gaussian with a width of the instrumental resolution. We find in Fig. 4 that the superconducting state measured along \( E_F \) near \( T_c^{opt} \) is a guide for the eyes.

Remarkably, when we normalize the wave vector so as to align the peak at \( E_F \) and the highest binding energy (250 meV), the dispersions near \( E_F \) show a systematic difference among three compounds as shown in Fig. 4(d). It is evident that the “kink” in dispersion becomes more pronounced as \( n \) increases. This observation strongly suggests that the coupling strength increases with the number of CuO\(_2\) layers in a unit cell and consequently the maximum \( T_c \). A similar behavior, indicative of the stronger coupling with larger \( n \), is also observed in the ARPES spectral line shape around the \( M \) point, where the “peak-dip-hump” structure becomes more pronounced with larger \( n \). This similarity in the \( n \) dependence suggests the same origin for the “kink” structure along the nodal direction and the “peak-dip-hump” around the \( M \) point in the superconducting state.

The results in Figs. 4 and 3(b) imply an important nature of the many-body effect in the low-energy excitations. We found that the coupling constant and the \( \Delta_{max} \) increase with increasing \( n \) (maximum \( T_c \)), pointing to a possible correlation between these two important physical parameters. Furthermore, the present ARPES result also puts a constraint on

\[ T_c \sim \frac{\Delta_{max}}{k_B T_c} \]

\[ \Delta_{max} \sim k_B T_c \]
interpreting a microscopic origin of the coupling between electrons and the collective mode. If the coupling is purely due to the longitudinal-optical phonon, the present ARPES result suggests that the phonon density of states (or dispersion) should show a systematic difference with \( n \), whereas the representative phonon frequencies look similar to each other (50–80 meV). On the other hand, if the coupling is from the magnetic mode, it is expected that the intensity of the resonance peak around \( Q = (\pi, \pi) \) in inelastic neutron-scattering (INS) experiments increases with increasing \( n \). Recently Kee et al. reported that the intensity of the magnetic-resonance peak is too small to account for the significant kink features observed by ARPES. If this is the case, it raises another question as to why the temperature dependence of the magnetic resonance peak around \( 50–80 \) meV closely resembles that of the kink features observed by ARPES. If this is the case, it raises another question as to why the temperature dependence of the magnetic-resonance peak closely resembles that of the

In conclusion, we have performed systematic high-resolution angle-resolved photoemission spectroscopy of Bi-family HTSCs. We have shown that the holelike Fermi surface and the \( d_{x^2-y^2} \)-like superconducting gap are generic features of the \( \text{Cu}_2 \) plane, irrespective of the number of layers in a unit cell. In addition, we have found a scaling rule in the doping dependence of the energy gap for three compounds. Comparison of the nodal dispersion in the superconducting state has also revealed that the interaction of electrons with mode is stronger for larger \( n \).

We thank M. Mori, T. Tohyama, J. R. Engelbrecht, and Z. Wang for useful discussions. This work was supported by a Grant-in-Aid for Scientific Research from MEXT of Japan, the U.S. National Science Foundation (NSF) Grant No. DMR-0072205, and the Sloan Foundation. T.S. thanks the Japan Society for Promotion of Science for financial support. The Synchrotron Radiation Center is supported by U.S. NSF Grant No. DMR-0084402.

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