Fermi surface and superconducting gap in superstructure-free $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$

T. Sato, T. Kamiyama, Y. Naitoh, and T. Takahashi
Department of Physics, Tohoku University, Sendai 980-8578, Japan

I. Chong, T. Terashima, and M. Takano
Institute for Chemical Research, Kyoto University, Uji 611-0011, Japan
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We report an ultrahigh-resolution angle-resolved photoemission spectroscopy on superstructure-free $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ with various hole concentrations. The Fermi surface retains a holelike character centered at (π, π) from under- to overdoping. The superconducting gap exhibits a $d_{x^2-y^2}$-like anisotropy with a typical gap value of 10–15 meV near $(\pi, 0)$. Comparison with $Bi_2Sr_2CaCu_2O_8$ shows that the size of the superconducting gap and the energy of the hump structure near E_F are well scaled with the maximum $T_c(T_c^{\max})$. This suggests that the superconducting properties are essentially characterized by $T_c^{\max}$ irrespective of the number of CuO_2 layers or the BiO superstructure.

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Angle-resolved photoemission spectroscopy (ARPES) has been intensively employed on $Bi_2Sr_2CaCu_2O_8$(Bi2212) and has revealed several important features of the cuprate high-T_c superconductors (HTSC's) such as the $d_{x^2-y^2}$-like superconducting gap[1–3] and the pseudogap above the superconducting transition temperature (T_c).[4–7] Detailed analysis of ARPES spectra has elucidated the interaction of electrons with a collective mode of wave vector (π, π).[8] On the other hand, a recent ARPES study on Bi-system HTSC's using higher photon energies has raised a question regarding the so-far believed holelike Fermi surface (FS) in HTSC's, proposing an electronlike FS centered at the (0, 0) point.[9] It is well known that Bi2212 has two CuO_2 layers per unit cell and also a strong incommensurate modulation in the BiO layer. It is still unknown how the double CuO_2 layers affect the electronic structure and consequently the superconducting properties. Further, the incommensurate superstructure in the BiO layer is expected to strongly modify the electronic structure and, in fact, complicates the interpretation of ARPES spectra.[9–11] In contrast to Bi2212, $Bi_2Sr_2CuO_6$ (Bi2201) has a single CuO_2 layer per unit cell, though a slight modulation in the BiO layer still remains. A recent structural study has found that substitution of Bi with Pb completely erases the superstructure in the Bi(Pb)O layer.[12] It is thus very important to perform ARPES measurements on Pb-substituted Bi2201 to check the universality of the key features observed so far in Bi2212 as well as to obtain an insight into the Fermi-surface topology free from the structural modulation.

In this paper, we report a systematic ultrahigh-resolution ARPES study on superstructure-free $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ with various dopings [underdoped (UD) $T_c = 18\,\mathrm{K}, 19\,\mathrm{K}$ to overdoped (OD) $T_c = 13\,\mathrm{K}, 0\,\mathrm{K}$]. We found that the FS retains its holelike character for all the doping levels from UD 18 K to OD 0 K. We have observed a $d_{x^2-y^2}$-like anisotropic superconducting gap. By comparing the present experimental results on Bi2201 with those on Bi2212, we found that the key superconducting properties observed so far in Bi2212 are essentially universal in the Bi-system HTSC's irrespective of the number of CuO_2 layers or the structural modulation in the BiO layer, and their characteristic energies are well scaled with the maximum T_c of each compound. In contrast, we have also observed that the ARPES spectral feature is less resolved in Bi2201 than in Bi2212 even when we take into account the scaling factor, which may suggest an intrinsic difference between the two compounds.

Single crystals of Pb-substituted Bi2201 ($Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$) were grown by the traveling-solvent floating-zone method.[12] The composition was determined by fluorescence x-ray analysis. We have confirmed by transmission electron microscopy that the crystals are free from any structural modulations.[12] The doping level was controlled by annealing under vacuum at high temperature of 500–600 °C. The T_c of samples was determined by the magnetic susceptibility measurement and is UD $T_c = 18\,\mathrm{K}, 19\,\mathrm{K}$ and OD $T_c = 13\,\mathrm{K}, 0\,\mathrm{K}$, where 0 K means that the sample does not show any signature of superconductivity down to 4 K. ARPES measurements were performed using a SCIENTA SES-200 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator. We used the He Iα resonance line (21.218 eV) to excite photoelectrons. The energy and angular (momentum) resolutions were set at 7–11 meV and 0.25° (0.01 $\mathrm{Å}^{-1}$), respectively. The Fermi level (E_F) of the sample was referenced to a gold film evaporated onto the sample substrate and its accuracy is estimated to be better than 0.4 meV.

Figure 1(a) shows the photoelectron intensity map along the $(\pi, 0)$-(π, π) cut at 13.5 K for four samples with different dopings. Figures 1(b) and 1(c) show a set of ARPES spectra of a UD 18-K sample measured along (0, 0)-$(\pi, 0)$ and (0, 0)-(π, π) cuts, respectively. It is clear from Fig. 1(a) that there is a dispersive feature near E_F centered at $(\pi, 0)$ that crosses E_F midway between $(\pi, 0)$ and (π, π) for all the samples. The Fermi momentum (k_F) determined by the $|\nabla_k n(k)|$ method[13] is shown by arrows for OD 0 K ($k_F = 0.1\pi$) and UD 18 K ($k_F = 0.15\pi$).[14] We find that the Fermi momentum is gradually shifted toward the (π, π) point when the doping level is decreased. On the other hand, we find in Figs. 1(b) and 1(c) that a band dispersing from (0, 0) to $(\pi,$

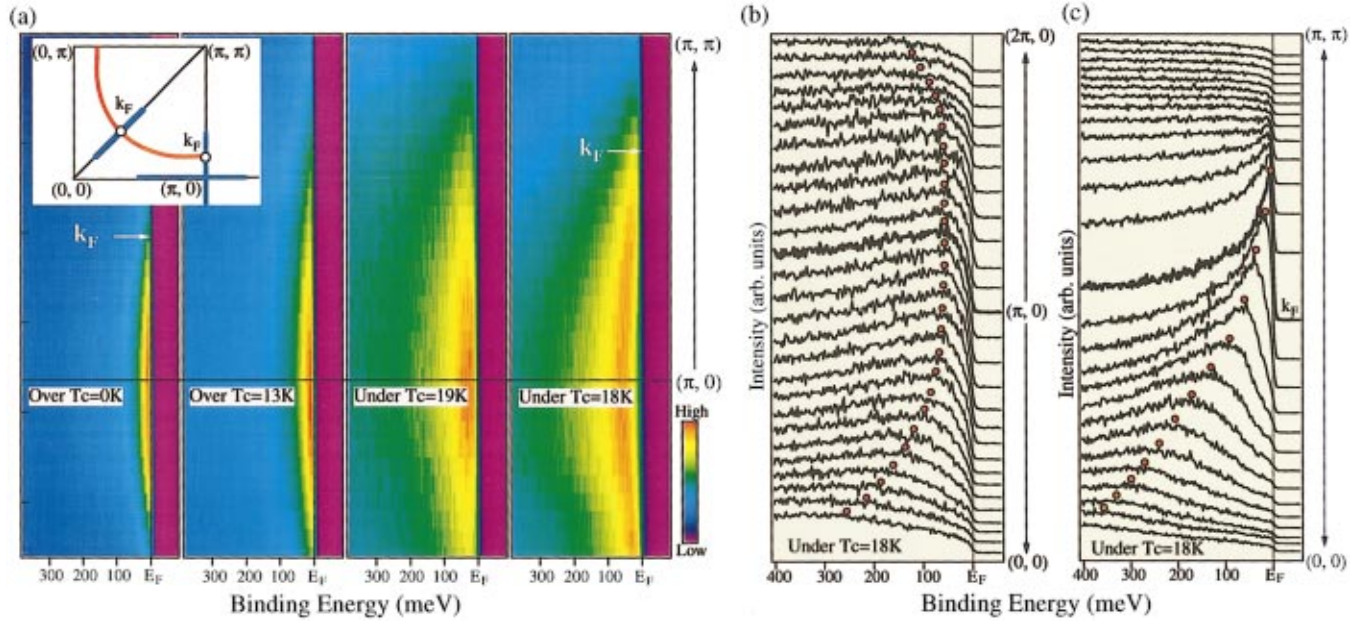

FIG. 1. (Color) (a) ARPES intensity map of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ for four samples with different dopings (overdoped $T_c=0$ K, 13 K to underdoped $T_c=19$ K, 18 K). Bright area corresponds to the high ARPES intensity. Vertical axis corresponds to the momentum along the $(\pi, 0)$-(π, π) cut while the abscissa shows the binding energy relative to E_F. The Fermi momentum (k_F) determined by the $|\nabla_k n(k)|$ method (Ref. 13) is shown by arrows for OD 0 K ($k_F=0.1\pi$) and UD 18 K ($k_F=0.15\pi$). The inset shows the Brillouin zone with a schematic Fermi surface obtained from the present measurement (red line) and three cuts where ARPES measurements were done. (b) ARPES spectra of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ (underdoped $T_c=18$ K) measured along the (0, 0)-$(\pi, 0)$ cut at 25 K. Rough peak position is indicated by red circles. (c) ARPES spectra of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ (underdoped $T_c=18$ K) measured along the (0, 0)-(π, π) cut at 13.5 K.

0) does not cross E_F while there is a single E_F crossing of the band in the (0, 0)-(π, π) direction. All these experimental results unambiguously indicate that there is a holelike FS centered at (π, π), in good agreement with previous reports,[15–17] and the volume of FS systematically changes with doping by keeping its holelike character for all the dopings from OD 0 K to UD 18 K. However, it is not clear at present whether the FS topology changes with photon energy as reported in Bi2212 (Ref. 9) since we used only one photon energy (He I, 21.218 eV) from a discharge lamp. A careful ARPES study with synchrotron radiation is necessary to clarify this.

Figure 2 shows ARPES spectra in the very vicinity of E_F measured at two k_F points along $(\pi, 0)$-(π, π) and (0, 0)-(π, π) cuts for an UD 19 K sample, compared with those of a gold-film reference. We find that the ARPES spectrum at the $(\pi, 0)$-(π, π) crossing shows a remarkable leading-edge shift relative to that of gold while the leading edge at the (0, 0)-(π, π) crossing almost coincides with the gold reference. This clearly indicates that an anisotropic $d_{x^2-y^2}$-like superconducting gap opens in Bi2201 as well as in Bi2212.[1–3] Referring to the temperature dependence of the superconducting gap of Bi2212,[18] it is expected that an almost full superconducting gap opens at 13.5 K in the present Bi2201 sample ($T_c=19$ K) because an almost full gap opens at 60 K in the Bi2212 sample with $T_c=90$ K.[18] In order to estimate the size of the superconducting gap, we have simulated the spectrum with the BCS spectral function by taking into account the finite-energy resolution and the finite temperature

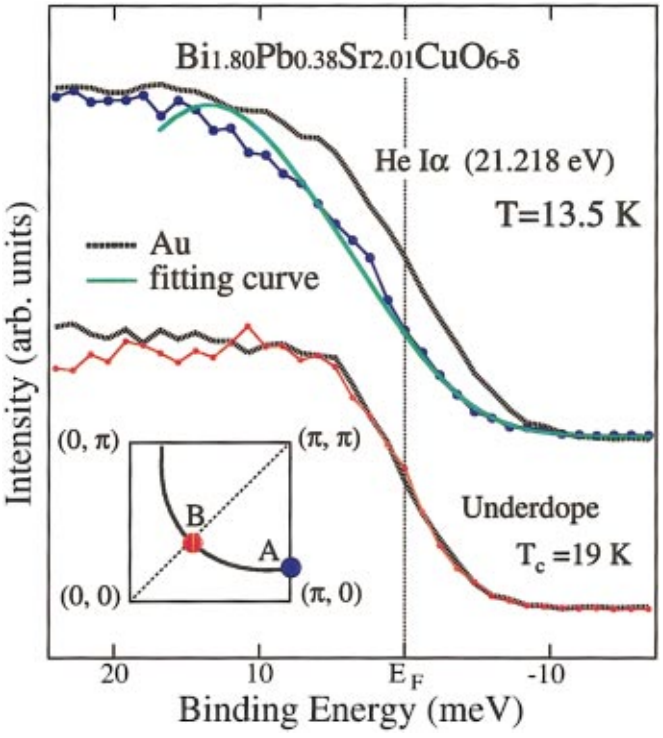

FIG. 2. (Color) ARPES spectra in the very vicinity of E_F measured at the Fermi momentum at 13.5 K along the $(\pi, 0)$-(π, π) and (0, 0)-(π, π) cuts for $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ (underdoped $T_c=19$ K) compared with those of a gold-film reference. A green line denotes the numerical simulation to estimate the superconducting gap. For details, see text.

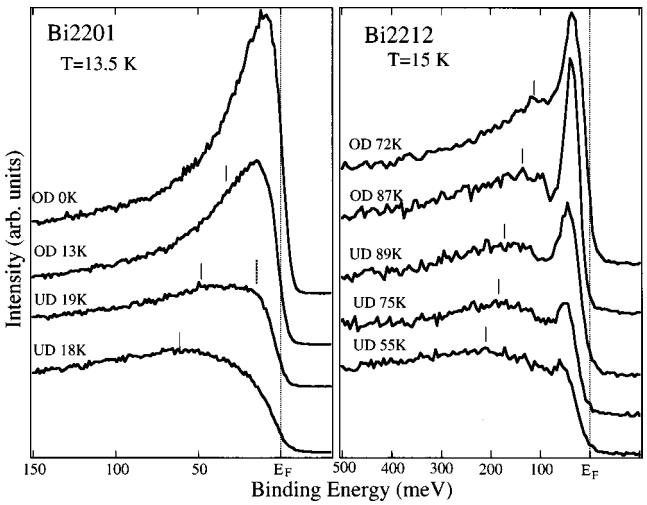

FIG. 3. Comparison of doping dependence of the ARPES spectrum at the $(\pi, 0)$ point between Bi2201 and Bi2212 (Ref. 8). Rough energy position of the hump structure is marked by bars. Broken bar in the ARPES spectrum of Bi2201 UD 19 K shows a possible position of the quasiparticle peak.

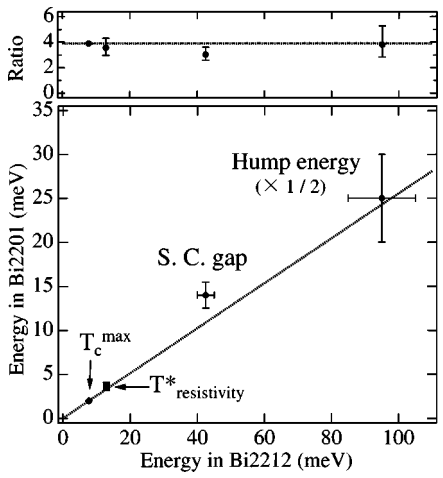

FIG. 4. Comparison of representative characteristic energies of superconducting properties [size of the superconducting gap, energy position of the hump structure in ARPES spectrum, and T^* at which the in-plane resistivity of the optimally doped sample shows a deviation from the T-linear behavior (Refs. 12 and 25)] between Bi2201 and Bi2212. A straight line shows the ratio of $T_c^{\max}$ of each compound [90 K (Bi2212)/23 K (Bi2201)=3.9]. Note that all the values are on/near this line, suggesting existence of an energy scaling between Bi2212 and Bi2201.

effect (Fermi-Dirac function at 13.5 K). The result is shown with the green line in Fig. 2. We find that the leading edge of the ARPES spectrum is well fitted by the simulation, while the higher-binding energy region is not well reproduced probably because the incoherent part and the background in the ARPES spectrum are not included in the simulation. The estimated gap size of the UD 19 K sample is 14 ± 1.5 meV. This value is relatively small compared with a typical value (40–45 meV) reported for Bi2212 with a similar hole concentration,[19–21] reflecting the difference in the T_c, namely, the strength of the pairing interaction. It is remarked here that the ratio of the gap size (40–45 meV/14 meV $=2.9-3.2$) is close to the ratio of the maximum $T_c(T_c^{\max})$ for each compound [90 K(Bi2212)/23 K(Bi2201)$\sim$3.9]. This suggests the existence of a certain scaling in the characteristic energy of the superconducting property.

Figure 3 shows the doping dependence of the ARPES spectrum at $(\pi, 0)$ for Bi2201 and Bi2212.[8] Detailed analysis of the ARPES spectra of Bi2212 in this momentum region has revealed the interaction of electrons with a collective mode.[8] For Bi2212 we clearly find a ''hump-dip-peak'' structure produced through this interaction in all the spectra from UD 55 K to OD 72 K. We find a small humplike structure around 50 meV in the spectra of UD 18 K and UD 19 K in Bi2201 as denoted by bars. This humplike structure may correspond to that around 200 meV in Bi2212. Further, a quasiparticlelike peak appears at about 20 meV in the spectrum of UD 19 K as shown by a broken bar. It is thus inferred that the overall ARPES spectral feature near E_F and its doping dependence are similar between Bi2212 and Bi2201, although the energy scale is distinctly different between the two. When we compare the energy scale between Bi2212 and Bi2201 from the energy position of the humplike structure in each ARPES spectrum (Bi2201 UD 19 K and Bi2212 UD 75 K), we obtain the ratio of 3.8 (=190/50). Surprisingly, this value is almost the same as that of the $T_c^{\max}$ ($\sim$3.9), suggesting existence of a certain energy scaling in the ARPES spectrum near E_F between Bi2201 and Bi2212. In spite of the similarity in overall structure in the ARPES spectrum near E_F, we find in Fig. 3 that the spectral feature is less resolved in Bi2201 than in Bi2212. This broad nature in the ARPES spectrum in Bi2201 is not understood even when we take into account the energy scaling ratio ($\sim$3.9) and/or the measurement temperature relative to the T_c. Referring to a previous ARPES study on Bi2212,[22] it is expected that the present energy resolution (7 meV) is sufficient to resolve each structure near E_F in Bi2201 as well as in Bi2212. It is also remarked here that a similar broad nature in the ARPES spectrum near E_F has been observed in other single-CuO_2 layer compounds such as $Bi_2Sr_{2-x}La_xCuO_{6+\delta}$,[17] $La_{2-x}Sr_xCuO_4$,[23] and $HgBa_2CuO_{4+\delta}$.[24] Therefore, the absence of a clear hump-dip-peak structure may be an intrinsic and common feature for single-layer compounds, although the origin is not clear at present, and this awaits further investigation.

Next we compare the various energy scales in Bi2201 and Bi2212. Figure 4 summarizes the comparison of characteristic energies of the superconducting properties (T_c, size of the superconducting gap, and energy of the hump in the ARPES spectrum) between Bi2201 and Bi2212. In Fig. 4 we also include the temperature at which the in-plane resistivity of the optimally doped sample shows a deviation from the T-linear behavior.[12,25] Since the in-plane resistivity is believed to be closely related to the pseudogap,[25] this temperature serves as a measure of temperature (T^*) at which a pseudogap opens at E_F, although the T^* was not determined in this study due to a fast degradation of the sample surface at high temperature. A straight line in Fig. 4 shows the ratio of $T_c^{\max}$ between Bi2212 (90 K) and Bi2201 (23 K). As seen

in Fig. 4, the size of the superconducting gap, the energy position of the hump structure in the ARPES spectrum, and T^* are well scaled with $T_c^{\max}$. This suggests that the superconducting and pseudogap properties are essentially the same in both Bi2212 and Bi2201 irrespective of the number of CuO_2 layers or the structural modulation in the BiO layer, and their characteristic energies are well scaled with the maximum T_c, namely, the strength of the pairing interaction. Finally we briefly comment on the collective mode in Bi2201. A recent theoretical work by Abanov and Chubukov[26] has shown that the energy separation between the peak and the dip at $(\pi, 0)$ in the ARPES spectrum corresponds to the energy of the collective mode of wave vector (π, π), which couples with electrons and leads to the superconductivity. Indeed, a recent precise ARPES study on Bi2212 has revealed the collective mode with the energy of $\sim$40 meV,[8] which shows a good agreement with the energy of the magnetic-resonance peak observed by neutron scattering on Bi2212.[27] In contrast to Bi2212, the ARPES spectrum of Bi2201 does not show a clear dip-peak structure (Fig. 4). However, considering the energy scaling in the ARPES spectrum at $(\pi, 0)$ (Fig. 4), the peak-to-dip separation in Bi2201 is expected to have a value smaller than that of Bi2212 by a factor of the ratio (3.9). This estimates a value of 10 meV for the mode energy in optimally doped Bi2201. A neutron-scattering experiment on Bi2201 is thus greatly desired to check the mode energy and consequently the energy scaling.

In conclusion, from the present ultrahigh-resolution ARPES study on superstructure-free Pb-substituted Bi2201 with various dopings, we found that (i) Bi2201 has a holelike Fermi surface centered at (π, π) in the entire doping region from UD 18 K to OD 0 K, (ii) the superconducting gap symmetry is $d_{x^2-y^2}$-like with a typical maximum gap value of 10–15 meV, and (iii) the ARPES spectral feature near E_F (hump-dip-peak structure) and its doping dependence of Bi2201 are similar to that of Bi2212 while the energy scale is remarkably different and the spectral feature is less resolved in Bi2201. By comparing the present results on Bi2201 with those on Bi2212, we found that the characteristic energies of the superconducting properties are well scaled with the maximum T_c ($T_c^{\max}$) of each compound. This suggests that the superconducting properties are characterized by $T_c^{\max}$ irrespective of the number of CuO_2 layers or the structural modulation in the crystal.

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