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Evidence for a hole-like Fermi surface of $Bi_2Sr_2CuO_6$ from temperature-dependent angle-resolved photoemission spectroscopy

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We report temperature-dependent angle-resolved photoemission spectroscopy (ARPES) on superstructure-free $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ (overdope, $T_c < 4$ K) to study the topology of the Fermi surface. The temperature dependence of ARPES spectra unambiguously shows the existence of a dispersive band that crosses E_F along the $(\pi,0)$-(π,π) cut, indicating a holelike Fermi surface centered at (π,π). We also found that the spectral intensity is strongly affected by k-dependent matrix elements but the spectral function itself suffers no photon-energy dependence.

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I. INTRODUCTION

The Fermi surface (FS), defined as a set of wave vectors (k) in momentum space at which an infinitely small energy is required to create electronic exitation, plays an essential role in characterizing the physical properties of solids. Since the topology of the FS is closely related to the transport and thermodynamic properties, the relation between the FS topology and the anomalous physical properties has been intensively discussed in many materials. Angle-resolved photoemission spectroscopy (ARPES) is a unique and powerful experimental technique to study the momentum-resolved electronic structure. By use of this unique capability, ARPES has elucidated the electronic band structure and the Fermi surface of many interesting materials. In fact, observation of a large holelike FS centered at (π,π) in high-T_c superconductors[1,2] (HTSC's) has served as an essential experimental basis for modeling the high-T_c mechanism. However, a recent ARPES study on $Bi_2Sr_2CaCu_2O_8$ (Bi2212) with higher-energy photons has raised a question on the holelike FS scenario, proposing an electronlike FS centered at (0, 0).[3] This proposal has stimulated many ARPES studies[4–12] with various different methods to determine the FS topology, but a final consensus has not yet been obtained.

One of main difficulties in precisely determining the Fermi-level crossing or the Fermi vector (k_F) by ARPES lies in the inherent nature of the photoemission process; photoemission spectroscopy probes only the occupied states. In ARPES, k_F is usually determined by finding a k point at which a peak in the ARPES spectrum dispersing toward E_F suddenly loses its intensity. This procedure has been widely used and proved to be very successful in the case where the band dispersion is experimentally well defined within the experimental (energy and momentum) resolution of ARPES. On the other hand, it has gradually become clear that this method has a limitation in the case where the peak is located very close to E_F with no substantial dispersion. The present controversy on the FS topology in Bi2212 is exactly the latter case; a very flat band close to E_F (extended Van Hove singularity) is situated around the $(\pi,0)$ point. As an alternative way to determine k_F precisely, several methods have been proposed, such as taking a maximum gradient of the momentum distribution function [$\nabla n(k)$ method][13] and plotting ARPES intensity at E_F as a function of k.[14] However, it is found that either is not decisive due to a considerable

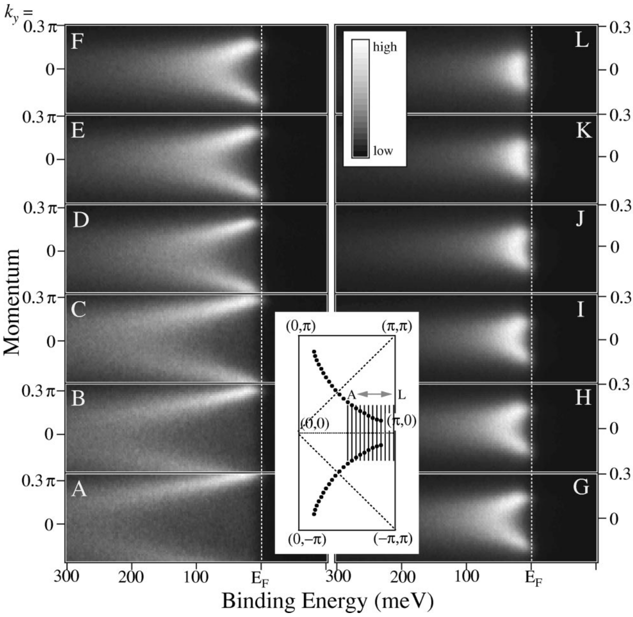

FIG. 1. ARPES intensity as a function of binding energy and momentum for $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ (T_c<4 K), measured at 25 K with 22-eV photons along several cuts parallel to (π,0)-(π,π) in the Brillouin zone (see inset). Filled circles in the inset show k_F's determined by the $\nabla n(k)$ method.

influence from the finite energy and momentum resolution as well as the dipole matrix element. It is also noted that the incommensurate superstructure in the BiO layer complicates the interpretation of ARPES data in Bi2212.[15,16]

In this paper we report a temperature-dependent ARPES study on superstructure-free Pb-substituted $Bi_2Sr_2CuO_6$ (Bi2201). The absence of a superstructure in the BiO layer removes the complication due to overlapping from umklapp bands in analyzing ARPES spectra. Further, the temperature dependence of ARPES spectra has unambiguously revealed the exact location (above or below E_F) of a band near E_F decisive for the determination of the FS topology.

II. EXPERIMENT

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.[17] The transmission electron microscopy confirmed no structural modulation in the crystal (BiO layer). The crystal does not show superconductivity down to 4 K, indicating the sample is overdoped due to Pb substitution.[17] ARPES measurements were performed using a GAMMADATA-SCIENTA SES200 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator, as well as at the undulator 4m-NIM beam line at Synchrotron Radiation Center in Wisconsin. We used He Iα (21.218 eV), 22 eV, and 28 eV photons to excite photoelectrons. The energy and angular (momentum) resolutions were set at 11–15 meV and 0.25 deg (0.01 Å^{-1}), respectively.

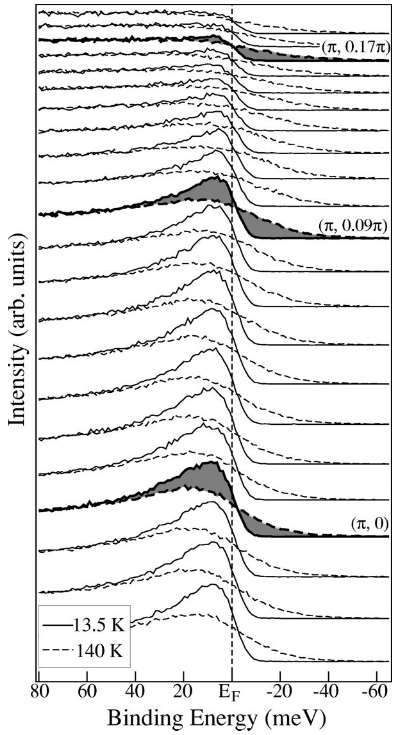

FIG. 2. ARPES spectra near E_F of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ measured with He Iα photons along the (π,0)-(π,π) cut at 13.5 K (solid lines) and 140 K (broken lines).

III. RESULTS AND DISCUSSION

In Fig. 1 we plot the ARPES intensity as a function of binding energy and momentum for $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ measured at 25 K with 22-eV photons along several cuts parallel to (π,0)-(π,π). It is at first noted that there is no additional peaks (bands) in this energy and momentum region in contrast to the Bi2212 case,[2–6,8–11] where several umklapp bands due to the BiO superstructure appear and overlap the main band. This clearly indicates that the present Bi2201 crystal is free from the superstructure and appropriate to study the genuine Fermi surface originating in the CuO_2 layer. As found in Fig. 1, the energy dispersion away from the (π,0) point is very steep and shows a clear Fermi-level crossing (k_F), indicating that the bottom of the band is actually located below E_F. When one approaches the (π,0) point, the band gradually becomes less dispersive and finally almost dispersionless around the (π,0) point. This indicates the existence of an extended Van Hove singularity (VHS) very close to E_F, commonly observed in hole-doped HTSC's. One of the key points to differentiate a holelike and an electronlike FS is the position of the band relative to E_F at the (π,0) point. If the band is located below E_F at (π,0), the topology is holelike and vice versa. However, it is not clear from Fig. 1 whether the band is located below or above E_F at the (π,0) point, although a nonzero ARPES intensity is seen below E_F, because the ARPES might see a thermally broadened tail of the band located above E_F. In order to clarify this point, we measured the temperature dependence of ARPES spectra in the (π,0)-(π,π) cut.

Figure 2 shows near-E_F ARPES spectra in the

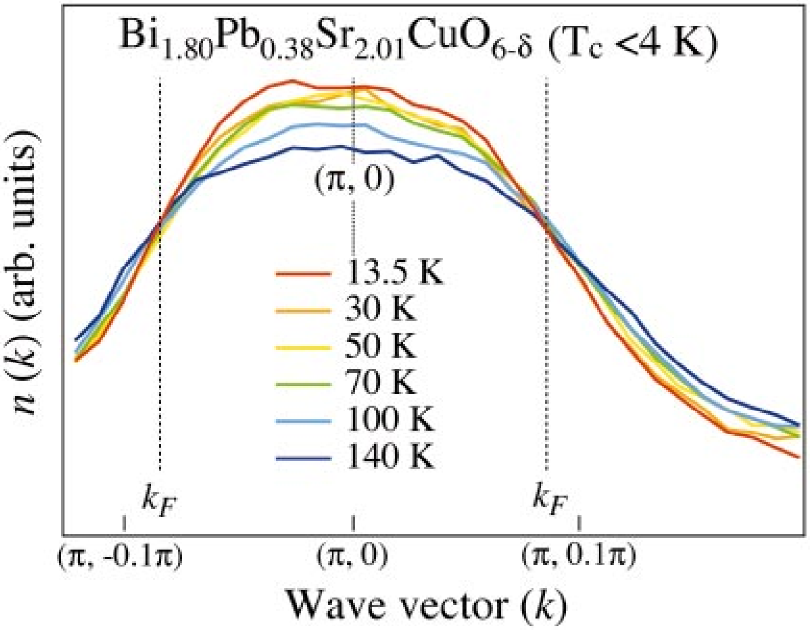

FIG. 3. (Color) Temperature dependence of integrated ARPES intensity $I(k)$ along the $(\pi,0)$-(π,π) cut, obtained by integrating ARPES intensity from 100 to -100 meV binding energy. The angle-integrated-type temperature-independent background is subtracted before integration.

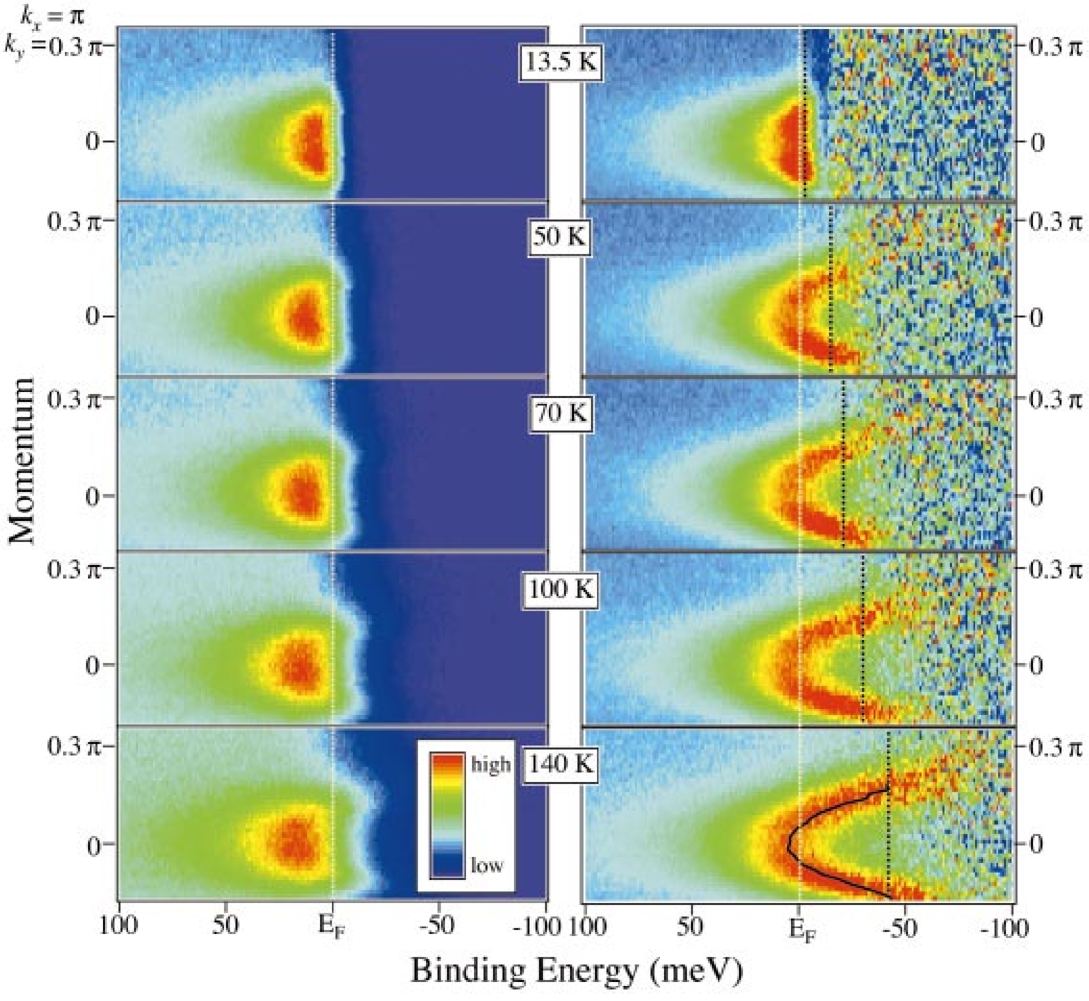

FIG. 4. (Color) Left panel: temperature dependence of ARPES intensity of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ along the $(\pi,0)$-(π,π) cut. Right panel: same divided by the FD function at each temperature convoluted by a Gaussian of a width of energy resolution (11 meV). Dotted lines show the energy above E_F at which the FD function takes a value of 0.03. The solid line in the 140-K data indicates the peak position obtained by fitting with a Lorentzian.

$(\pi,0)$-(π,π) cut measured at two different temperatures, 13.5 and 140 K. Spectral intensity is normalized to the area under the curve from 100 to 200 meV binding energy (not shown in Fig. 2), where we expect a negligible change of the Fermi-Dirac (FD) function in the temperature range of 13.5–140 K. The spectrum of 13.5 K at $(\pi,0)$ shows a sharp peak at E_F, which gradually reduces its intensity on approaching (π,π) without any remarkable change of the peak position. Thus it is not clear from only the 13.5 K-spectra whether the band is below or above E_F at the $(\pi,0)$ point. In contrast, spectra at 140 K are significantly broadened due to the temperature (FD function) effect. We clearly find a transfer of spectral weight from below to above E_F on increasing temperature, as shown by the shaded area, because the FD function at 140 K has a wider tail above E_F. A key point in the present temperature-dependent ARPES is that the total spectral weight does not seem to conserve at each k point. For example, ARPES spectrum at $(\pi,0)$ looks to lose the total intensity at 140 K since the increased volume above E_F seems smaller than the decreased counterpart below E_F, while a totally opposite behavior is observed at $(\pi,0.17\pi)$. This apparent peculiar temperature dependence of ARPES intensity is understood in terms of the redistribution of electrons obeying the temperature-dependent FD function and is potentially used to determine precisely the k_F point, as demonstrated by previous works.[13,18] It is noted here that the total ARPES intensity should conserve at k_F.[13]

In order to determine k_F precisely, we show in Fig. 3 the temperature-dependent integrated ARPES intensity $I(k)$ obtained by integrating intensity from 100 to -100 meV. $I(k)$ corresponds to $M(k)n(k)$, where $M(k)$ is the momentum-dependent dipole matrix element term and $n(k)$ is the momentum distribution function. The obtained $I(k)$ shows a maximum intensity at $(\pi,0)$ in each temperature and gradually decreases on approaching (π,π). An important finding in Fig. 3 is that $I(k)$ at $(\pi,0)$ monotonously decreases with increasing temperature while $I(k)$ substantially away from the $(\pi,0)$ point increases at the same time. The $I(k)$ is found to be constant with temperature at a midpoint denoted by the broken line. According to the discussion above, this point is identified as the k_F point along the $(\pi,0)$-(π,π) cut, indicating that the band is below E_F at the $(\pi,0)$ point. This clearly shows that Pb-substituted Bi2201 (overdope, $T_c<4$ K) has a holelike FS centered at (π,π). The k_F from $(\pi,0)$ is estimated to be $(\pi,0.085\pm0.01\pi)$.

The holelike FS in overdoped Bi2201 is also confirmed by a different method with the same ARPES data. Photoemission spectroscopy basically probes only the occupied part of electronic states due to the cutoff by the temperature-dependent FD function. In reverse, by using the tail of the FD function above E_F, we can investigate the electronic states slightly above E_F together with the states below E_F, as demonstrated by Greber *et al.* for Ni.[19] Figure 4 shows the ARPES intensity along the $(\pi,0)$-(π,π) cut divided by the FD function at each temperature convoluted by a Gaussian with a width of energy resolution (11 meV). The raw ARPES-intensity plot is also shown for comparison. In contrast to the raw ARPES data, those divided by the FD function show the band dispersion slightly above E_F. It is remarked here that the dispersion above E_F is more clearly seen at higher temperature, because the tail of the FD function extends more above E_F at higher temperature. As described above, the importance of distinguishing the FS topology is whether the bottom of the band at $(\pi,0)$ is located below or above E_F. We have performed numerical fitting to the FD-function-divided ARPES spectra with a single Lorentzian and found that the bottom of the dispersive band is located at about 5 meV below E_F as shown by a solid line in the 140-K data. The k_F estimated by the fitting is $(\pi,0.075\pm0.01\pi)$ in good agreement with the estimation from the temperature-dependent ARPES in Fig. 3. The same fit gives about 150 meV Å dispersion at the Fermi surface along the $(\pi,0)$-(π,π) direction.

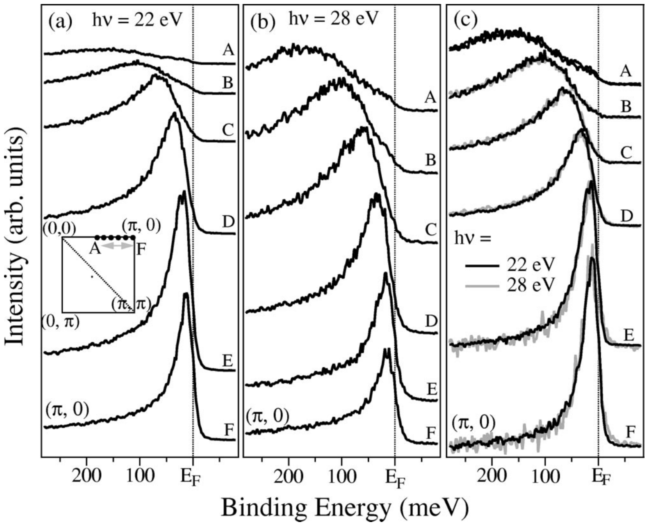

FIG. 5. ARPES spectra of $Bi_{1.80}Pb_{0.38}Sr_{2.01}CuO_{6-\delta}$ along the (0,0)-$(\pi,0)$ cut measured with (a) 22-eV and (b) 28-eV photons. (c) A comparison of both sets of ARPES spectra after subtracting the background and scaling the intensity.

The next important problem to be solved is whether the FS topology is photon-energy dependent or not, as presently discussed in Bi2212.[1–12,16] Figures 5(a) and 5(b) show ARPES spectra along the (0,0)-$(\pi,0)$ cut measured with 22- and 28-eV photons, respectively. In contrast to the 22-eV spectra, the ARPES intensity at 28 eV is substantially suppressed around the $(\pi,0)$ point, as in Bi2212 around 33 eV,[3,4,7,9,11] suggesting an E_F crossing of the band midway between (0, 0) and $(\pi,0)$ and as a result an electronlike FS centered at (0, 0). However, we found that ARPES spectra measured at the same k point with different photon energies (22 and 28 eV) are essentially identical after subtracting the background and scaling the intensity, as shown in Fig. 5(c). This indicates that the spectral function itself suffers no photon-energy dependence, but the dipole matrix element term considerably modifies the spectral intensity. The present ARPES result thus unambiguously shows that the FS of Bi2201 is holelike centered at (π,π) independently of the incident photon energy. Further it is naturally expected that optimally or underdoped Bi2201 also has a similar holelike FS with a smaller volume,[20] although it is not finally excluded that a more heavily overdoped sample may have an electronlike FS as in $La_{2-x}Sr_xCuO_4$ (LSCO).[21,22]

IV. CONCLUSIONS

We have performed temperature-dependent ARPES on superstructure-free Pb-substituted $Bi_2Sr_2CuO_6$ and shown that the overdoped Bi2201 ($T_c < 4$ K) has a holelike Fermi surface centered at (π,π). We also found that the spectral function itself suffers no photon-energy dependence, but the dipole matrix element term considerably modifies the spectral intensity.

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