

Electron-Like Fermi Surface and Remnant ($\pi,0$) Feature in Overdoped $\text{La}_{1.78}\text{Sr}_{0.22}\text{CuO}_4$

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INTRODUCTION

Studies of the Fermi surface in the high temperature superconductors by angle resolved photoemission spectroscopy (ARPES) have mostly been focused on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ (BSCCO)[1-6]. In this system, however, additional features, such as the Bi-O superstructures in BSCCO, have made the analysis rather complicated. $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ (LSCO), by virtue of the absence of these effects and the availability of high quality single crystal samples over the entire doping range, provides the opportunity to advance our understanding of the high temperature superconductors. In the overdoped regime, an electron-like Fermi surface was observed in the high- T_c superconductors for the first time[7], but despite this progress, important problems remain. Since ARPES data from underdoped samples are very broad, worries about the sample quality persist. There are also questions about the effects of the photoemission matrix element[8], which makes it difficult to extract quantitative information about stripe effects on nodal spectral weight. We address these important questions by performing a detailed study of overdoped LSCO ($x=0.22$). Our detailed analysis shows that the compound has an electron-like Fermi surface with additional spectral weight near $(\pi,0)$, which is the remnant of the flat band feature in the underdoped samples.

EXPERIMENT

The ARPES measurements were carried out at BL10.0.1.1 of the Advanced Light Source, using incident photons with an energy of 55.5 eV. We used a SCIENTA SES-200 spectrometer in angle mode, where one can collect spectra over ~ 14 degrees, corresponding to a momentum width of $\sim 1.1\pi$ (in units of $1/a$, where $a \sim 3.8\text{\AA}$ is the lattice constant). The total energy and momentum resolution was about 20 meV and 0.02π , respectively. We studied high quality single crystals of LSCO with $x=0.22$ grown by the traveling-solvent floating-zone method. The measurements were performed in an ultra high vacuum of 10^{-11} Torr at 20 K and the samples were cleaved *in situ*. The position of the Fermi level (E_F) was calibrated with gold spectra.

RESULTS AND DISCUSSION

Figure 1 shows the spectral weight plot integrated over a 30 meV window around the Fermi level [(a),(c)] for two geometries and simulations of the spectral weight plot for each geometry including transition matrix element effects [(b),(d)] (see below). Integrating over the narrow window of the order of the energy resolution makes it possible to obtain the spectral weight at E_F , which approximately represents the Fermi surface. The Fermi surfaces at $k_z = 0$ and π/c from the band-structure calculation for $\text{La}_{2-x}\text{M}_x\text{CuO}_4$ ($x = 0.2$) [9], as well as the Fermi surface from the present tight-binding fit are superimposed on Fig. 1(a). As a whole, they well describe the global features related to the Fermi surface obtained from ARPES. The volume enclosed by the tight-binding Fermi surface satisfies Luttinger's sum rule within experimental accuracy.

Here, we have performed simulations of spectral weight distribution including matrix-element effects by using the same method described in [10,11]. As shown in Fig. 1(b), in geometry I, the nodal states in the first BZ show almost no spectral weight while those in second BZ are enhanced, consistent with the experimental data in Fig.1(a). This implies that the suppression in geometry I compared to geometry II is caused by matrix element effects. According to the simulation, the enhancement in the second BZ may be caused by the angular distribution factor of the three atomic orbitals, because they have a small emission probability for small angles when the E -vector is vertical to the surface. The simulation in Fig. 1(d) shows an enhancement of the spectral weight in the $(0,0)$ - (π,π) direction compared to the nodal states of the first BZ in geometry I, which qualitatively agrees with the experimental results.

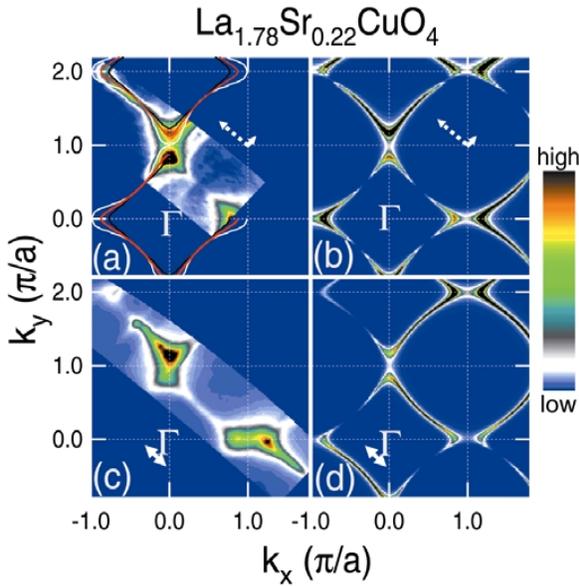


Figure 1. Spectral weight integrated within 30 meV of the Fermi level. White arrows designate the E vector. (a)(c); Experiment. (b)(d); Simulation. White and black curves in (a) represent the Fermi surfaces of band calculation[9] at $k_z=0$ and π/c , respectively, and red curves represents the Fermi surface from the present tight-binding fit. Note that the spectral weight in the nodal direction is enhanced for geometry II [(c) and (d)] compared to geometry I [(a) and (b)].

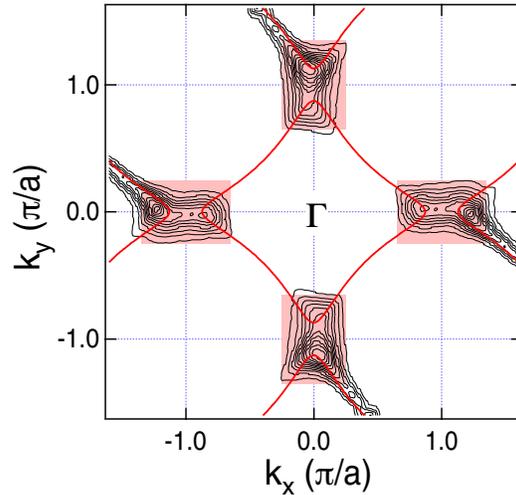


Figure 2. Contour plot of the spectral weight shown in Fig. 1(c) symmetrized with respect to the Γ point. Red curves show the electron-like Fermi surface obtained from the fit to the energy dispersion results. Shaded regions around $(\pi, 0)$ reflect a remnant of the “flat band”.

While the overall features in the experimental results agree with the simulation as shown above, there was still a discrepancy between them regarding the spectral weight distribution near $(\pi,0)$. As shown in Fig. 2, the spectral weight distribution around $(\pi,0)$ shows a relatively straight contour along the k_x direction, which is slightly narrower than that in Nd-LSCO ($|k_y| < \pi/4$) [12]. This spectral weight distribution is very similar to that of the flat band which appears below E_F for smaller x . Presumably the $(\pi,0)$ flat band feature which exists in the optimum and underdoped regions does not completely lose its spectral weight even for $x=0.22$ where the saddle point is located above E_F . Therefore, the spectral weight around $(\pi,0)$ appears as a remnant of the “flat band”. In the case of BSCCO, the possibility of additional states at $(\pi,0)$ has been proposed [1]. Figure 4 illustrates that the present results may be described by an electron-like Fermi surface feature and a remnant feature of the “flat band”.

CONCLUSION

In conclusion, we have unambiguously observed an electron-like Fermi surface in slightly overdoped LSCO $x=0.22$, which agrees with the band-structure calculation. By utilizing the matrix element effects, we have obtained clear dispersion and sharp peak features for the nodal states comparable to BSCCO. The transition matrix element effects have been discussed by simulations, which account for the enhancement in the second BZ and for different geometries. The spectral weight around $(\pi,0)$, which may be interpreted as a remnant of the “flat band”, is discussed.

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