ELSEVIER

Physica C 341–348 (2000) 2087–2090

PHYSICA C

www.elsevier.nl/locate/physc

ARPES Features of the AF Insulators $Sr_2CuO_2Cl_2$ and $Ca_2CuO_2Cl_2$ Close to the AF Zone Boundary

F. Ronning[a*], C. Kim[a], A. Damascelli[a], N. P. Armitage[a], D.H. Lu[a], K. M. Shen[a], L.L. Miller[b], Y.J. Kim[c], M.A. Kastner[c], R.J. Birgeneau[c], and Z.-X. Shen[a]

[a]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University, Stanford, CA 94305, USA
[b]Department of Physics, Iowa State University, Ames, IA 50011, USA
[c]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

ARPES studies on $Sr_2CuO_2Cl_2$ and $Ca_2CuO_2Cl_2$ are presented. The integrated spectral weight of the low energy feature shows a drop across the AF zone boundary, suggesting a remnant Fermi surface. Along the remnant Fermi surface the dispersion fits the functional from of $|\cos(k_x a) - \cos(k_y a)|$ remarkably well. However, additional experiments with improved angular resolution demonstrate that the dispersion near $(\pi/2, \pi/2)$ does not contain a cusp as would be expected from a simple d-wave theory predicting the above functional form. The rounded node region and the total dispersion of approximately 350meV is shown to be independent of photon energy.

1. Introduction

In order to understand the physics of the high T_c cuprates, particularly on the underdoped side, we must understand how a hole behaves amidst antiferromagnetic correlations. Considering this, it is desirable to study the electronic structure of the parent compounds using Angle Resolved Photoemission(ARPES). This technique is ideal since by ejecting an electron from the undoped sample, one is examining the motion of a single hole in an AF insulator. This reasoning motivated the earlier ARPES work on $Sr_2CuO_2Cl_2$(SCOC) and $Ca_2CuO_2Cl_2$(CCOC), both of which have a Neel temperature close to 250K[1][2].

The spectra on the insulator reveal a well defined, although broad, feature with a minimum binding energy at $(\pi/2, \pi/2)$. The spectra from (0,0) to (π, π) look remarkably similar to that of hole doped $Bi_2Sr_2CaCuO_{8+\delta}$(BSCCO) samples, with the obvious exception that the insulating features do not reach the chemical potential[1]. The recent work on CCOC mapped out the features over the entire Brillouin zone [2]. The dispersion is approximately 350meV and isotropic about $(\pi/2, \pi/2)$. A remnant Fermi surface was identified and a d-wave like feature was observed along it, lending support to the notion that the high energy pseudo gap and the insulator feature as seen by photoemission have the same origin[3].

2. Experimental

The CCOC measurements were conducted at Beamline V-3 of the Stanford Synchrotron Radiation Laboratory (SSRL). The angular resolution was $\pm 1°$. SCOC measurements were performed at beamline V-4 of SSRL where the angular resolution used was 0.25°. The samples were oriented prior to the experiment by the Laue method and were cleaved *in situ*. The chamber pressure was better than $5 \times 10^{-11} torr$. Data were taken in the $\vec{k}$-space octant $(0,0) - (\pi,0) - (\pi,\pi) - (0,0)$ and well below the Neel temperature of $250K$. Since the samples are insulating, charging of the sample during the measurement can be a concern. By varying the photon flux we are able to ensure that the samples are not charging. Since CCOC and SCOC are isostructural with almost identical lattice parameters one would expect the physics of these 2 materials to be the same[4]. Indeed the only difference noticed by photoemission is

*Email: fronning@leland.stanford.edu

PII S0921-4534(00)01090-X

that CCOC has slightly more spectral weight at $(\pi, 0)$ compared to SCOC. This difference made it possible to observe the remnant Fermi surface in CCOC when it had not previously been identified in SCOC.

3. $n(\vec{k})$

The spectra of CCOC shows a small foot on the low binding energy side of the valence band. As in the case of the hole doped materials, this low energy feature is believed to originate from the Zhang-Rice singlet of the CuO_2 planes. Figure 1 shows the intensity of the low energy feature from a CCOC sample over a quarter of the Brillouin zone. The relative $n(\vec{k})$ was determined by integrating the low energy feature over a 700meV window. The graph has been symmeterized about $k_x = k_y$ for illustrative purposes, the crosses indicate the locations in k-space where spectra have been taken, and a linear interpolation was used to derive the observed contours. The photon energy used was 25.2eV. Unfortunately, ARPES measures the convolution of the single particle excitation spectrum, $A(\vec{k}, \omega)$ and the matrix element[5]. In some sense, the matrix element can be thought of as external factors which enter through the measurement process which obscure the determination of $A(\vec{k}, \omega)$. This includes factors such as the experimental geometry and the polarization of the incident beam[6]. Keeping this in mind one is still able to identify a remnant Fermi surface, and it is marked by the hashed lines in the figure. The reason for this identification is that the loss of spectral weight in the low energy feature roughly along the AF zone boundary, running from $(\pi, 0)$ to $(0, \pi)$, bears a striking similarity to the $n(\vec{k})$ pattern seen in optimally doped BSCCO[2]. It also roughly coincides with the LDA prediction for the Fermi surface in this material[7]. Perhaps the most interesting feature of the remnant Fermi surface is that along it the dispersion fits the simple d-wave form of $|\cos(k_x a) - \cos(k_y a)|$ remarkably well. (Although certainly not a trivial result, we will refer to "simple" d-wave theories as those which predict the dispersion to be the functional form above.) The experimental dispersion can be seen in Figure 2 by the filled squares. However, this result does open a few questions. Theoretically, one must wonder about the significance of such a good fit to the d-wave-like form in the insulator. Furthermore, the data begs the question of whether or not the dispersion truly exhibits a cusp at the node region. Any d-wave theory predicts four nodes which will occur at 45° with respect to the Cu-O bond direction. With greatly improved angular resolution in ARPES over the past couple of years we can now address the latter question experimentally.

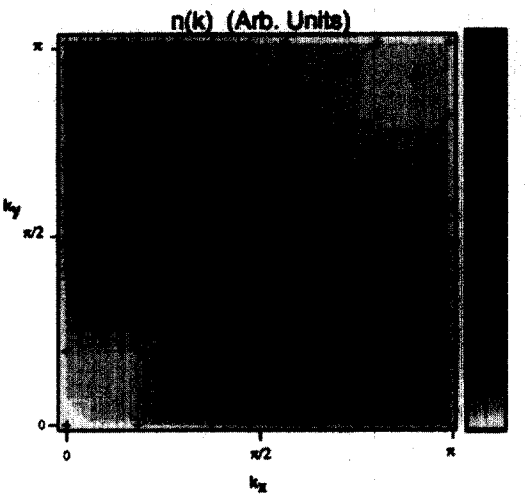

Figure 1. Two fold symmeterized scale plots of $n(\vec{k})$ of a CCOC sample taken with a photon energy of 25.2eV. The only drop in intensity which can not be explained by matrix element effects is the one indicated by the hashed lines. This is identified as the remnant Fermi surface. The crosses indicate where actual spectra were taken.

4. Rounded Node

Using a spectrometer with much better angular resolution(0.25°) we were able to take data with improved momentum resolution. The

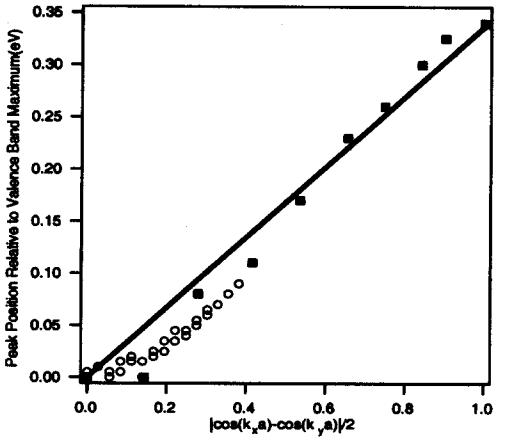

Figure 2. Dispersion of the insulator along the remnant Fermi surface. The solid squares are earlier CCOC data taken with angular resolution of ±1°[2]. The open circles are SCOC data taken with 0.25° resolution. The fit to a simple d-wave function is good, but the data indicates an unexpected flattening of the dispersion near $(\pi/2, \pi/2)$.

filled squares in Figure 2 show the peak position relative to the valence band maximum of a CCOC sample taken with relatively poor angular resolution(±1°). The data is taken roughly along the AF zone boundary and is plotted against the function $|\cos(k_x a) - \cos(k_y a)|/2$. A simple d-wave theory on this plot would give a straight line through the origin such as the one shown. Even with the poor angular resolution one can see that the data hints that the node region is rounded[2]. Also included in the figure is data from a SCOC sample, shown with open circles taken with a newer spectrometer which allows for the much improved momentum resolution. From this it becomes clear that the node region is indeed rounded. It is apparent that the simple d-wave picture although a good fit, will not fit the data in the node region.

In the past the flattening of the superconducting or pseudo gap dispersion has been compared with a dirty d-wave picture[8]. Although it is still possible that impurities are responsible for the rounding observed here, there are several reasons to believe that this is not the case. Results on underdoped BSCCO show that the superconducting gap becomes more rounded in the node region as the system approaches the insulator[9]. The fact that the rounding seen in CCOC is greater than that seen in their most underdoped sample agrees with this trend. Also, SCOC and CCOC are very chemically stable compounds as evidenced by the inability to dope them. We would also like to mention that, although not shown here, data taken on CCOC with improved momentum resolution also shows a rounded dispersion about $(\pi/2, \pi/2)$.

5. Photon Energy Dependence

Recently, ARPES data on cuprates has seen a surprising dependence on photon energy. Using a photon energy of 32eV an electron like Fermi surface centered about (0,0) was observed in BSCCO[10]. This contradicted most other work, which was performed with photon energies at or below 22eV, and claim to see a hole pocket centered at (π, π)[11]. This contradiction is particularly surprising because the electronic structure of the cuprates is generally believed to be 2 dimensional. As a result, ARPES spectra should show no photon energy dependence. Why then would two different photon energies result in two different scenarios? One possible explanation is that the low energy ARPES spectra are composed of multiple features which have different cross-sectional dependencies on the photon energy. Alternatively, perhaps the difference is due to a lack of appreciation for possible effects due to the 3 dimensionality of these materials. The matrix element is surely to come into question as well. It is apparent that the photon energy dependence of the cuprates should be more closely examined.

Thus, to gain more insight into the problem, we have studied the photon energy dependence of the ARPES spectra of the AF insulator. Figure 3 shows the dispersion of CCOC along the rem-

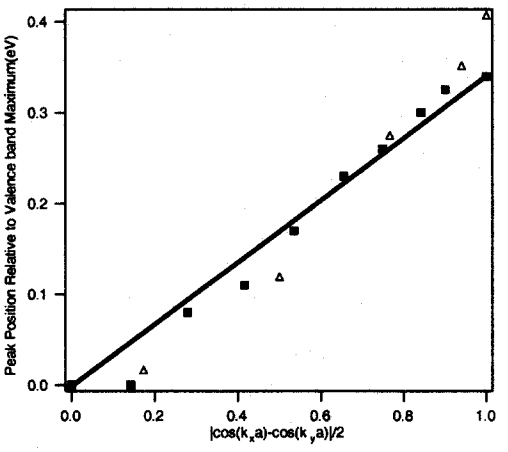

Figure 3. Similar to Figure 2, the dispersion of the insulator along the remnant Fermi surface is plotted. The solid squares are identical to those in Figure 2, and indicate CCOC data which was taken using 25.2eV photons. The open triangles are CCOC data taken with 33eV photons. Both still show a good fit to the simple d-wave prediction, and no photon energy dependence of the dispersion is observable.

nant Fermi surface taken at two different photon energies. The only difference in experimental conditions between the two sets of data is that the solid squares were taken at 25.2eV while the open triangles were take with 33eV photons. As would be expected for a 2 dimensional system, there is no difference between the dispersion found at the two different photon energies. There is even still the indication of the rounded node region in both cases.

6. Conclusions

The insulator shows the intensity of the low energy feature to lose weight as one approximately crosses the AF zone boundary. Along the zone boundary, a d-wave-like dispersion exists; however, near the node region of $(\pi/2, \pi/2)$ a simple d-wave theory is unable to account for the rounding of the dispersion. The dispersion is independent of photon energy as would be expected assuming that the system is 2 dimensional.

7. Acknowledgements

This work was performed at the Stanford Synchrotron Radiation Laboratory which is supported by the DOE Office of Basic Energy Science, Divisions of Chemical Sciences and Material Sciences. It is also supported by the ONR grant N00014-98-1-0195 and NSF grant DMR-9705210.

REFERENCES

1. B.O. Wells *et al.*, Phys. Rev. Lett. **74** 964 (1995); S. LaRosa *et al.*, Phys. Rev. B **56** R525 (1997); J.J.M. Pothuizen *et al.*, Phys. Rev. Lett. **78** 717 (1997); C. Kim *et al.*, Phys. Rev. Lett. **80** 4245 (1998).
2. F. Ronning *et al.*, Science **282**, 2067 (1998).
3. R.B. Laughlin, Phys. Rev. Lett. **79** 1726 (1997).
4. L.L. Miller *et al.*, Phys. Rev. B **41** 1921 (1990).
5. S. Hufner, Photoelectron Spectroscopy (Springer-Verlag, Berlin, 1995).
6. A. Bansil and M. Lindroos, Phys. Rev. Lett. **83** 5154 (1999).
7. D.L. Novikov *et al.*, Phys. Rev. B **51** 6675 (1995).
8. J.M. Harris *et al.*, Phys. Rev. B **54** R15665 (1996); A. Loeser *et al.*, Science **273**, 325 (1996).
9. J. Mesot *et al.*, Phys. Rev. Lett. **83** 840 (1999).
10. N.L. Saini *et al.*, Phys. Rev. Lett. **79** 3467 (1997); Y.-D. Chuang *et al.*, Phys. Rev. Lett. **83** 3717 (1999).
11. Z.-X. Shen and D.S. Dessau, Phys. Rep. **253** 1 (1995); H. Ding *et al.*, Phys. Rev. Lett. **76** 1533 (1996); Fretwell *et al.*, cond-mat/9910221; S.V. Borisenko *et al.*, cond-mat/9912289.