Lawrence Berkeley National Laboratory
LBL Publications

Title

Constancy of the bilayer splitting as a function of doping in $Bi_{2}Sr_{2}CaCu_{2}O_{8+δ}$

Permalink

https://escholarship.org/uc/item/2212r28n

Authors

Chuang, Y-D
Gromko, AD
Fedorov, AV
et al.

Publication Date

2001-06-29

Peer reviewed

eScholarship.org Powered by the California Digital Library
University of California

arXiv:cond-mat/0107002v2 [cond-mat.supr-con] 6 Jul 2001

Constancy of the bilayer splitting as a function of doping in $Bi_2Sr_2CaCu_2O_{8+\delta}$

Y. -D. Chuang[1,2], A. D. Gromko[1], A.V. Fedorov[1,2], Y. Aiura[3], K. Oka[3], Yoichi Ando[4], D. S. Dessau[1]

[1]*Department of Physics, University of Colorado, Boulder, Colorado 80309-0390*

[2]*Advanced Light Source (ALS), Berkeley, CA 94720*

[3]*National Institute for Advanced Industrial Science and Technology (AIST) AIST Tsukuba Central, 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568,Japan*

[4]*Central Research Institute of Electric Power Industry (CRIEPI), 2-11-1 Iwato-Kita, Komae, Tokyo 201-8511, Japan*

(Received November 16, 2017)

Abstract

Using high energy resolution angle resolved photoemission spectroscopy, we have resolved the bilayer splitting effect in a wide range of dopings of the bilayer cuprate $Bi_2Sr_2CaCu_2O_{8+\delta}$. This bilayer splitting is due to a nonvanishing intracell coupling $t_\perp$, and contrary to expectations, it is not reduced in the underdoped materials. This has implications for understanding the increased c-axis confinement in underdoped materials.

Typeset using REVTEX

It has long been thought that the high temperature superconducting cuprates can to first order be treated as two dimensional systems since the transport properties within the ab-plane (CuO_2 plane) and along the c-axis are very different. Such anisotropy shows up for example in the resistivity ratio $\rho_c/\rho_{a,b}$ and their temperature dependence $\rho_{(a,b),c}(T)$ [1,2]. Other probes such as the optical conductivity and interlayer tunneling measurements also indicate that the charge transport along the c-axis is severely reduced, especially in underdoped samples [3,4]. This leads to the general notion that the physics of these materials is almost entirely two dimensional, and can be well described by a single CuO_2 plane. However, this picture seems to be incompatible with the fact that the transition temperature T_c is closely related to the number of CuO_2 planes per unit cell [5], with single layer compounds of a family generically having lower T_c's than bilayer or trilayer compounds. Additionally, recent experiments on the organic-chain intercalated $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) showed that isolated CuO_2 planes do not possess superconductivity [6]. These results highlight the importance of the c-axis couplings for the superconductivity. Therefore, although they have been largely neglected so far, it appears clear that studies of the c-axis coupling effects on the electronic structure will be critical for a clear understanding of the high T_c phenomenon.

A large advance was made recently by angle-resolved photoemission (ARPES) experiments on the overdoped bilayer cuprates $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) which showed for the first time the existence of the normal state c-axis intracell coupling [7,8]. The coupling between adjacent CuO_2 planes within the bilayer, $t_\perp$, was observed as a splitting of the near Fermi energy (E_F) bands into a Bonding (B) and Antibonding (A) set. This effect was found to be maximal at the $(\pi, 0)$ point of the zone and to go to zero along the $(0,0)-(\pi,\pi)$ nodal line, consistent with theoretical predictions [9]. The extracted coupling value $t_\perp$ of $55meV$ is reduced from band theory predictions by about a factor of 3, indicating sizable correlation effects.

Considering the highly unusual physics in the underdoped regime including in particular the pseudogap [10] and the non-Fermi liquid behavior due to some sort of increased correlations [11], it is natural to wonder whether the correlations which reduce $t_\perp$ are enhanced in

the underdoped regime as well. General expectations are that they would, since (1) the c-axis conductivity (DC [1] and optical conductivity [4]) is greatly reduced in the underdoped samples, indicating greater two dimensional confinement, (2) correlations are expected to be stronger as the parent Mott insulator is approached, and (3) the bilayer splitting has not yet been directly observed in the underdoped regime. In this letter, we present the first direct evidence that bilayer splitting exists generically in the Bi2212 family irrespective of doping, and in fact, the energy splitting is essentially constant as a function of doping.

We performed high resolution ARPES on $Bi_2Sr_2CaCu_2O_{8+\delta}$ over a wide range of doping from heavily overdoped (OD, $T_c = 55K$), through optimal (OpD, $T_c = 91K$) and underdoped (UD, $T_c = 78K$), where the doping levels corresponding to different oxygen concentrations were achieved by high temperature anneals [12]. The experiments were carried out at the Advanced Light Source (ALS), Berkeley using the HERS Scienta endstation at the undulator BL10.0.1. Experimental details can be found elsewhere [13]. An important aspect of the experiments was the choice of photon energy, which we found adjusts the relative intensities of the bonding and antibonding bands, allowing an easier experimental deconvolution of the various features.

Figure 1 shows experimental spectra along the $(\pi, 0) - (\pi, \pi)$ line (green line of the Brillouin zone in panel (g), which also shows a schematic of the bonding FS (red) and antibonding FS (black)) [14]. False color images of the energy and momentum spectra along this cut are shown in panels (a)-(f) for the three dopings and for two photon energies ($22eV$, $47eV$). The bilayer-split bands labeled A and B are seen very clearly in panel (a) (OD, $22eV$), in the (red) energy distribution curve (EDC) in panel (h) and (red) momentum distribution curve (MDC) in panel (i). In the OpD and UD samples however, the intrinsic linewidth of the individual features is increased to a value equivalent to or even greater than the bilayer splitting energy, effectively masking the splitting.

Additional insight can be obtained by using the complementary photon energy of $47eV$, which we empirically found enhances the antibonding band A relative to the bonding band B (see panels (b), (h) and (i)). A recent first-principles calculation of the photoemission

matrix elements has independently shown this same effect [15]. Aside from the matrix element effect changing the intensity ratio of the two bands, we find that the lineshape and energy/momentum position of the A band is to within experimental uncertainty unchanged. This large matrix element modulation allows us to deconvolve the contribution from each of the bilayer-split bands in the optimal and underdoped samples, where the broadening of the individual features is relatively large.

Similar to what we have observed in panels (a) and (b), the $47eV$ images of (d) and (f) show a larger concentration of spectral weight near E_F than do the $22eV$ images of (c) and (e). This is seen more clearly in the EDCs at $(\pi, 0)$ shown in (j) and (l) which show a sharper feature at $47eV$(blue) than at $22eV$(red). We argue that this is because the $47eV$ data shows significant weight from the A band, while the 22 eV data additionally shows weight from the B band. The MDCs at E_F (panel (i), (k) and (m)) tell a similar story - the $47eV$ data is more concentrated at $k_y = 0.0$ corresponding to the A band, while the $22eV$ data extends farther out in $\vec{k}$ space because it contains weight from the B bands as well.

Figure 2 shows the Fermi Surfaces plots extracted from the data, including the effects of superstructure bands and some photon energy dependences. Panels (a) -(f) show the the locus of normalized near-E_F (in $\pm 10meV$ window) spectral weight throughout much of the Brillouin zone for the same OD and OpD samples and photon energies as in figure 1. The data were taken in the normal state ($T = 80K$ for OD and $100K$ for OpD and UD) and the $\vec{k}$ space location is indicated by the green box in panel (g). A few of the additional superstructure bands possible are also indicated in panel (g) [16]. Modulo matrix element effects which may be significant, the high intensity locus of this data should represent the Fermi Surface topology [17].

As in figure 1, the bilayer splitting is most clear in panel (a) of figure 2 (OD, $22eV$) where we see the A (black) and B bands (red) plus some of their superstructure replicas (light black and red lines). Also similar to figure 1, the $47eV$ data emphasizes the A band and so panel (b) (OD, $47eV$) almost exclusively shows the A band with a great amount of weight near $(\pi, 0)$ (in fact the matrix elements at $47eV$ favor the second zone somewhat,

causing the high weight portion to be slightly off of the $(\pi, 0)$ point). Panels (d), (f) show the FS topology very similar to that in (b), i.e. they all show the A FS topology. Panels (c) and (e) at $22eV$ are dominated by the standard hole-like FS corresponding to the B band.

The above data is relevant for the issue of the Fermi Surface topology of Bi2212, which has been an intensely debated issue recently. In particular, there has been a discussion about whether the Fermi Surface may sometimes (depending upon photon energy) exhibit a more electron-like character [20] , or whether there is a single unchanging hole-like piece plus superstructures, with no effects other than matrix elements which vary as a function of photon energy [21]. Figures 1 and 2 show that both FS topologies can be seen on any one sample depending upon the photon energy used, and this can be clearly understood to be simply due to the bilayer splitting effect. We believe that this should close the debate of the possibility of two types of Fermi Surfaces in Bi2212- they both exist. Whether one, the other, or both are observed depends upon the matrix elements which naturally vary with photon energies [22].

We note that the current data can not explicitly determine which side of $(\pi, 0)$ the antibonding band crosses, as it approaches exceedingly close to this point (this is the reason for the shading in panel (g) of figures 1 and 2). In other words, the van Hove singularity of the antibonding band is very near the Fermi level at this point. Typical notion is that if the band crosses E_F along $(0, 0) - (\pi, 0)$ line, the van Hove singularity is above the E_F whereas if it crosses along $(\pi, 0) - (\pi, \pi)$ then it is below E_F. In general it had been known that the van Hove singularity was near E_F, with a well known parameterization being $34meV$ below E_F [23]. While this is quite near E_F, it is still much larger than the temperature scale of T_c. On the other hand, the current data indicates that for the overdoped sample the antibonding band is at binding energy $9 \pm 2meV$ at the $(\pi, 0)$ point, which is comparable to the temperature scale of the problem [24]. This implies it should be quite active electronically. The van Hove singularity of the standard "hole-like" Fermi Surface (bonding component) is on the other hand about $100meV$ below E_F, making it much less relevant. This is important, as there have been many theoretical suggestions that a van Hove

singularity near E_F may be critical to understand the physics of these compounds [25–27] .

The existence of the bilayer splitting and its effect on the Fermi Surface topology is qualitatively new and was obtained directly from the raw data with no fitting or modeling required. This is the ideal most trustworthy case. There is much new quantitative information as well, and this can be extracted through a simple fitting of the data. Near E_F where the dispersion is steep we fit each set of MDCs with two Lorentzian peaks and a linear background (see for example figures 3(a)-(d)). Near the bottom of the bands where the dispersion is flat we fit the EDCs with two Lorentzian peaks plus a linear background multiplied by a Fermi cutoff (figure 3(e)-(g)). Usually we can only fit a portion of the spectra (positive k_y portion in (a), negative k_y in (b),(c),(d)) because of contamination by superstructure bands. The easiest data to fit is $22eV$ OD, which shows both A and B bands clearly and well separated (figure 3(a) and 3(e)). However, data from the optimal and underdoped samples can also be well fit if we tune to $47eV$ and use two bands A and B. It is much more difficult or impossible to fit these spectra with one peak [28].

The overall fitting results are compiled in figures 3(h) - 3(k), each set of which corresponds to about 20 fits of the type in panels (a)-(g). These were each taken along a cut about 27% of the zone away from $(\pi, 0)$ where the superstructure contamination was minimal ($k_x = 0.73\pi$ for $22eV$ data and 1.27π for $47eV$ data). The open circles are the EDC peak centroids and the closed circles are the MDC peak centroids. The dashed lines are quadratic fits to the centroids, implying a simple parabolic band dispersion [30]. The fact that both the MDC and EDC centroids are very well fit by the same parabolic bands gives high confidence for the quality of the data and fits for all sample types.

Panels (i) - (k) show the parabolic fits from all three sample types measured under identical conditions ($47eV$, $k_x = 1.27\pi$ cut, normal state). While the different doping levels give an energy offset of the parabolas from one sample to another ($30meV$ from OD to OpD and another $10meV$ from OpD to UD) due to the band filling effect, the shape and energy splitting of the parabolic curves are essentially unchanged with doping. In practice, we found the shape and splitting ($\approx 70meV$) of the parabolic curves from the OD sample

and then overlaid this parabola (shifted in energy but with the same splitting) with the data for the other samples. The good agreement is clear from the fits.

The bilayer splitting as a function of k has been theoretically parameterized as $\Delta(\vec{k}) = 0.5t_{\perp}(cos(k_x a) - cos(k_y a))^2$, which is zero along the node lines and maximal at the $(\pi, 0)$ points [9]. Using this formula to extrapolate the current data to $(\pi, 0)$ we get a maximum splitting of $114meV \pm 8meV$ or a $t_{\perp} \approx 57meV \pm 4meV$, obtained from the $47eV$ data. The $22eV$ data shown here (panel (h)) gives an estimate of $54meV$ also. This is in excellent agreement with our previous estimate of $55meV$ obtained on $25eV$ data [7]. Thus we conclude that $t_{\perp}$ is independent of the incident photon energies and has at the most a very weak dependence on the doping level.

The conclusion that $t_{\perp}$ depends weakly on the hole doping levels is quite surprising since the normal state resistivities show very different behavior, both in the magnitude and the temperature dependence [1,2]. For example, in the UD regime, ρ_c shows insulating behavior while ρ_{ab} is still metallic. In contrast, both ρ_{ab} and ρ_c are metallic in the overdoped regime. This type of data has been widely taken to indicate an increased two-dimensional confinement in the underdoped samples, a phenomenology that would be consistent with other exotic behaviors such as spin-charge separation [29] or marginal Fermi Liquid behavior [11]. While coupling between the unit cells is also relevant for the confinement, this coupling should be much weaker than the bilayer coupling discussed here, and in fact this coupling has not yet been directly observed. Our data directly implies a lack of increase in two dimensional confinement from the strong intracell $t_{\perp}$ and hints at a lack of change from the intercell $t_{\perp}$ effect. We suggest that other factors such as the increase in the scattering rate near $(\pi, 0)$, the onset of the pseudogap, or carrier fractionization should be more responsible for these anomalies in the transport behavior.

We acknowledge sample preparation help from J. Koralek and M. Varney and beamline support from S. Kellar, X.J. Zhou, P. Bogdanov, and Z. Hussain. This work was supported by the NSF Career-DMR-9985492 and the DOE DE-FG03-00ER45809. ALS is operated by the DOE, Office of Basic Energy Sciences.

REFERENCES

[1] T. Watanabe, T. Fujii and A. Matshda, Phys. Rev. Lett. **79**, 2113 (1997).

[2] Y. Ando *et al.*, Phys. Rev. Lett. **77**, 2065 (1996).

[3] C.E. Gough *et al.*, cond-mat/0002246.

[4] A.V. Puchkov, D.N. Basov and T. Timusk, J. Phys: Condens Matter **8**, 10049 (1996); A.V. Puchkov *et al.*, Phys. Rev. Lett. **77**, 3212 (1996).

[5] J.M. Tarascon *et al.*, Phys. Rev. B **38**, 8885 (1992).

[6] Mun-Seog Kim *et al.*, Phys. Rev. B **63**, 092507 (2001).

[7] Y.-D. Chuang *et al.*, cond-mat/0102386.

[8] D.L. Feng *et al.*, Phys. Rev. Lett. **86**, 5550 (2001).

[9] S. Chakravarty *et al.*, Science **261**, 337 (1993); O.K. Anderson *et al.*, J. Phys. Chem. Solids **56**, 1573 (1995).

[10] For review, see T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999); B. Battlogg and C. Varma, p. 33, Physics World, Feb 2000.

[11] C.M. Varma *et al.*, Phys. Rev. Lett. **63**, 1996 (1989).

[12] OD samples with a T_c of $55K$ were obtained by annealing as grown crystals at $T = 400^oC$ under a pressurized ($\gtrsim$ 1000 atm) Oxygen atmosphere; OpD samples with a T_c of $91K$ were obtained by annealing at $T = 700^oC$ in air and UD samples with a T_c of $78K$ were annealed in a reduced Oxygen atmosphere (400 torr Argon/100ppm Oxygen) at $T = 400^oC$.

[13] Y.-D. Chuang *et al.*, Science **292**, 1509 (2001).

[14] The EDCs used in making such plots were obtained in the normal state and were normalized by using high harmonic emission above E_F, which is believed to be isotropic

in momentum space.

[15] A. Bansil, private communication, SNS Conference, Chicago, IL, May 2001.

[16] These are due to the 5x1 superstructure modulation along the b or $\Gamma - Y$ axis.

[17] For example, see P. Aebi *et al.*, Phys. Rev. Lett. **72**, 2757 (1994).

[18] the red curves are the hole-like Fermi surface topology taken from ref [19]. The thick red lines are the main Fermi surface and the thin red lines are the Fermi surface from the lattice distortions (superstructure bands).

[19] H.Ding *et al*, Phys. Rev. Lett. **76**, 1533 (1996).

[20] Y.-D. Chuang *et al.* Phys. Rev. Lett. **83**, 3717 (1999); D.L. Feng *et al.*, cond-mat/9908056; P.V. Bodganov *et al.*, cond-mat/0005394.

[21] S.V. Borisenko *et al.*, Phys. Rev. Lett. **84**, 4453 (2000); M.S. Golden *et al.*, cond-mat/9912332; H.M. Fretwell *et al.*, Phys. Rev. Lett. **84**, 4449 (2000).

[22] A.D. Gromko *et al.*, to be published.

[23] M.R. Norman *et al.*, Phys. Rev. B **52**, 615 (1995).

[24] The curves at $k_x = 1.0$ were fit in a similar way to the data of figure 3.

[25] R.S. Markiewicz, J. Phys. Chem. Solids **58**, 1179 (1997).

[26] A.A. Abrikosov, Physica C **341-348**, 97 (2000)

[27] D. Newns *et al.*, Phys. Rev B **38**, 7033(1988); Phys. Rev B **43**, 3075(1991).

[28] The feature observed in UD sample at $47eV$ does show the superconducting gap of $\approx 35meV$ when we cooled down to $T = 30K$ which indicates its relavance to superconductivity. Data is not shown here.

[29] *THE Theory of Superconductivity in the High-T_c Cuprates* edited by P.W. Anderson,

Princeton Series in Physics, Princeton University Press, 1997.

[30] We note that in the normal state near the $(\pi, 0)$ point there is no clear mass renormalization or "kink".

FIGURES

FIG. 1. (a)-(f) Energy and momentum spectra along the $(\pi, 0) - (\pi, \pi)$ line, with a false color intensity scale. (g) A Fermi Surface plot indicating the location of the data cuts (green lines). Superstructure bands are not shown, and the shading near $(\pi, 0)$ indicates the uncertainty of the FS location. (h),(j),(l) EDCs at the $(\pi, 0)$ point. (I),(k),(m) MDCs at E_F. Red curves are $22eV$ data and blue curves are $47eV$ data.

FIG. 2. Integrated spectral weight over $(-10meV, 10meV)$ binding energy window. (a) OD,$h\nu = 22eV$. (b) OD, $47eV$. (c) OpD, $22eV$. (d) OpD, $47eV$. (e) UD, $22eV$. (f) UD, $47eV$. The shaded area of 1(g) is removed in these panels. (g) schematic FS topology with A FS (black) and B FS (red), plus a few of the SS bands (lighter).

FIG. 3. Fitting results on the $47eV$ data at $k_x = 1.27\pi$ and on the $22eV$ data at $k_x = 0.73\pi$. (a)-(d) Overlay of MDC at E_F with fitted curves. (e): Overlay of EDC at $(0.73\pi, 0.1\pi)$ at $22eV$ with fitted curves. Open circles are the data, dashed lines are Lorentzian peaks, dotted lines are the backgrounds and solid lines are the overall fitting results. (f),(g) Overlay of EDCs at $(1.27\pi, -0.1\pi)$ with fitted curves. (h) -(k) Overlay of the centroids from EDCs (open circles) and MDCs (closed circles) with parabolic fitting curves (dashed lines).