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Normal-state Fermi surface of pristine and Pb-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ from angle-resolved photoemission measurements and its photon energy independence

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We address the question as to whether the topology of the normal-state Fermi surface of $Bi_2Sr_2CaCu_2O_{8+\delta}$—as seen in angle-resolved photoemission—depends on the photon energy used to measure it. High-resolution photoemission spectra and Fermi-surface maps from pristine and Pb-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ are presented, recorded using both polarized and unpolarized radiation of differing energies. The data show clearly that no main band crosses the Fermi surface along the $\Gamma\bar{M}Z$ direction in reciprocal space, even for a photon energy of 32 eV, thus ruling out the existence of a Γ-centered, electronlike Fermi surface in this archetypal high-T_C superconductor. The true topology of the normal-state Fermi surface remains that of holelike barrels centered at the X,Y points of the Brillouin zone.

There is currently an ongoing and lively discussion regarding the true topology and character of the normal-state Fermi surfaces (FS's) of the high-temperature superconductors (HTSC's) in general, and of Bi2212 in particular. The "traditional" picture seen in angle-resolved photoemission spectroscopy (ARPES) is that of three different features with different origins: the main FS centred around the $X(Y)$ points[1] of the Brillouin zone (BZ), as predicted by band-structure calculations;[2] the so-called shadow FS due to antiferromagnetic spin correlations;[3] and extrinsic features [diffraction replicas (DR's)] which result from a diffraction of the outgoing photoelectrons as they pass through the structurally modulated Bi-O layers.[4]

Recently, ARPES data recorded with photon energies of 32–33 eV seemed to show a different picture and have been interpreted in terms of an electronlike FS centered around the Γ point.[5–7] It has even been suggested that the ARPES-derived FS depends on the photon energy used in the experiment.[6] This, of course, would constitute a revolution in our thinking about the normal-state FS's of the HTSC's and thus it is of utmost importance that this question be addressed quickly and clearly by a number of independent groups. In this contribution, we present ARPES investigations of Bi2212, with the aim of clearing up the controversy regarding the apparent photon energy dependence of normal-state FS topology as seen by photoemission.

We present a combination of energy distribution curves (EDC's) measured using polarized synchrotron radiation with angle-scanned photoemission data using unpolarized radiation at various photon energies and demonstrate that, as physical intuition dictates, the main FS of the Bi2212 materials is *independent* of the photon energy used to measure it in an ARPES experiment.

The synchrotron-based data were recorded using the U2-FSGM beamline at the BESSY I facility, with a sample temperature of 100 K, an overall energy resolution of 70 meV, and an angular resolution of $\pm 1°$, which gives $\Delta\mathbf{k} \leqslant 0.094$ Å^{-1} (i.e., 8.1% of ΓX) in the case of 32 eV radiation. In all cases the crystals were aligned such that the high-symmetry direction being scanned was parallel to the electric-field vector of the incoming synchrotron radiation. For the ΓY scans the analyzer was then swung downwards out of the plane spanned by the surface normal and the E vector, while for the $\Gamma\bar{M}Z$ scans the energy analyzer remained in the aforementioned plane. The angle-scanned ARPES experiments were performed at 300 or 120 K using monochromated, unpolarized He I and He II radiation and a SCIENTA SES200 analyzer enabling simultaneous analysis of both the E and $\mathbf{k}$ distribution of the photoelectrons. The overall energy resolution was set to 30 meV and the angular resolution to $\pm 0.38°$, which gives $\Delta\mathbf{k} \leqslant 0.028$ Å^{-1} (i.e., 2.4% of ΓX) in the case of He I radiation. High quality single crystals of pristine[8] and Pb-doped Bi2212, the latter grown from the flux in the standard manner, were cleaved *in situ* to give mirrorlike surfaces.[9]

Returning to the current ARPES controversy, certain points are universally accepted. First, there is a consensus that the traditional FS picture is correct for ARPES data recorded with low photon energies ($h\nu \leqslant 22$ eV).[6,10] Second, with respect to the high-symmetry directions in $\mathbf{k}$ space, the main FS crossing along the ΓX direction is also generally accepted to be valid for all photon energies used to date. Thus it is in fact the exact situation around the $\bar{M}$ point which is central to the debate, as it is in this region of $\mathbf{k}$ space where the closing of the main FS arcs to give a Γ-centered (electronlike) FS has been proposed.[5,6]

Consequently, in order to investigate the validity of this different FS topology in detail, as well as to address the question as to whether the final states (17–20 eV above E_F)

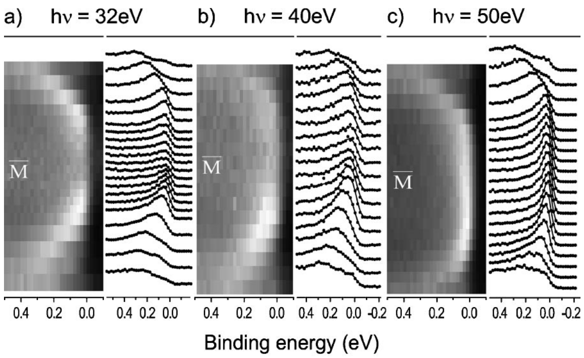

FIG. 1. ARPES of Bi2212 recorded at 100 K along the ΓM direction in **k** space for the photon energies: (a) 32 eV, (b) 40 eV, and (c) 50 eV. For each photon energy, the right panels show the spectra and the left panels $(E,\mathbf{k})$ plots in which the photoemission intensity is represented by a (linear) grey scale. For (a) the displayed region in **k** space goes from 0.19 up to 1.42 $Å^{-1}$, for (b) from 0.13 to 1.36 $Å^{-1}$ and for (c) from 0.24 to 1.45 $Å^{-1}$.

accessed with lower photon energies are in some way unrepresentative, we have measured EDC's of Bi2212 using synchrotron radiation of different energies along the $\Gamma\bar{M}Z$ line in **k** space. The data are shown in Fig. 1. For $h\nu=32$ eV, the $\Gamma\bar{M}$ data are very similar to those reported in Ref. 5, having been recorded in the same experimental geometry. In particular, the reduction of spectral weight around $\bar{M}$ for $h\nu=32$ eV, and to a lesser extent for 40 eV photons, could indeed be seen as a sign of a FS crossing, followed by the reappearance of the band between $\bar{M}$ and Z. However, a reduction of the spectral weight of the states related to the extended saddle-point singularity around $\bar{M}$ for $h\nu$ around 30 eV has been predicted to be due to matrix element effects alone in a recent theoretical treatment.[11] Furthermore, for $h\nu=50$ eV, the situation resembles that at lower photon energies and thus we see no indication of a $\Gamma\bar{M}$ FS crossing.

Since it is the $h\nu=32$ and 40 eV data which most significantly deviate from the commonly accepted picture, we devote the rest of the paper to their detailed discussion. The claims for a $\Gamma\bar{M}Z$ main FS crossing have been based not only on the intensity suppression around $\bar{M}$ as seen in Fig. 1, but also on an analysis of the **k** dependence of both the total photoemission intensity [which is related to the momentum distribution $n(\mathbf{k})$] and of the magnitude of the ARPES intensity at the Fermi level $[I(E_F)]$.[5] Figure 2(a) shows data for $h\nu=32$ eV for both the ΓY (panel 1) and $\Gamma\bar{M}$ (panel 2) directions. We start with the uncontroversial ΓY direction. The gray-scale image and $I_{int}/I(E_F)$ analysis shown in the panels marked 1 contain the signature of a main FS crossing—with a *sharp* peak in $I(E_F)$ coinciding with a *steep* drop in I_{int}. However, the analogous data for the $\Gamma\bar{M}$ direction [Fig. 2(a), panels marked 2] show a different behavior: both the drop in the total ARPES intensity as well as the peak in $I(E_F)$ are considerably broader than their counterparts along ΓY. In particular, the $I(E_F)$ peak is more than a factor of 3 broader than was the case for the ΓY main FS crossing. The question then arises as to whether this $I_{int}/I(E_F)$ characteristic for $\Gamma\bar{M}$ ($h\nu=32$ eV) is compatible with a *main* FS crossing. We believe that it is not, and will lay out our arguments for this in the following.

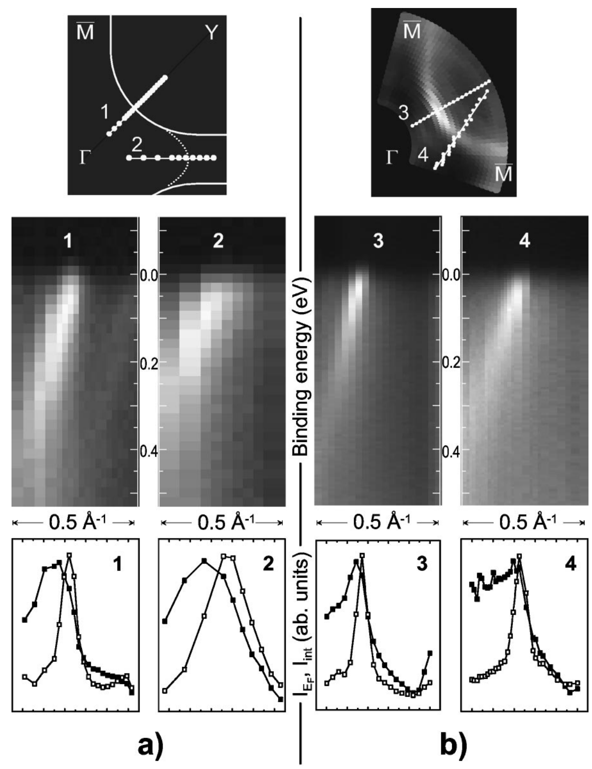

FIG. 2. (a) ARPES data from Bi2212 recorded with $h\nu=32$ eV at 100 K. (b) ARPES data from Pb-doped Bi2212 recorded with $h\nu=21.2$ eV at $T=120$ K. The chains of circles on the (a) BZ sketch and (b) FS map indicate the points in **k** space in which the ARPES data were measured. In the BZ sketch (a), the conventional and unconventional FS topologies are marked by solid or dotted white lines, respectively. Below the ARPES images (the linear grey scale indicates the intensity) is shown the analysis of the total photoemission intensity [I_{int}: solid squares, related to the momentum distribution $n(\mathbf{k})$] and the intensity in a 40 meV window centered on E_F [$I(E_F)$: open squares]. All panels have the same momentum scale.

First, assuming for the sake of argument the validity of the Γ-centered FS, the data for ΓY and $\Gamma\bar{M}$ both represent scans crossing the FS at right angles [see the sketch at the top of Fig. 2(a)]. Why, then, should the I_{int} and $I(E_F)$ analyses for the two directions be so different?

One argument that immediately springs to mind is based upon the fact that the photoemission features along the two directions [directly seen as white features in the $I(E,\mathbf{k})$ images of Fig. 2(a)] have different dispersion relations, thus possibly leading to the anomalous width in both I_{int} and $I(E_F)$ for $\Gamma\bar{M}$. A stringent test of this argument would be to compare the $\Gamma\bar{M}$ data with the $I_{int}/I(E_F)$ characteristics of a band, which not only crosses the main FS at right angles, but also displays the *same* dispersion relation as that observed along $\Gamma\bar{M}$ for $\mathbf{k}\leqslant\mathbf{k}_F$. Ideally speaking, this test should also be carried out for $h\nu=32$ eV, but in practice this is hampered by severe difficulties in the location of a true right-angular FS crossing, which could not, of course, be along a high-symmetry direction. This last point means that additional complications in the quantification of I_{int} and $I(E_F)$ would also result from the strong matrix-element effects im-

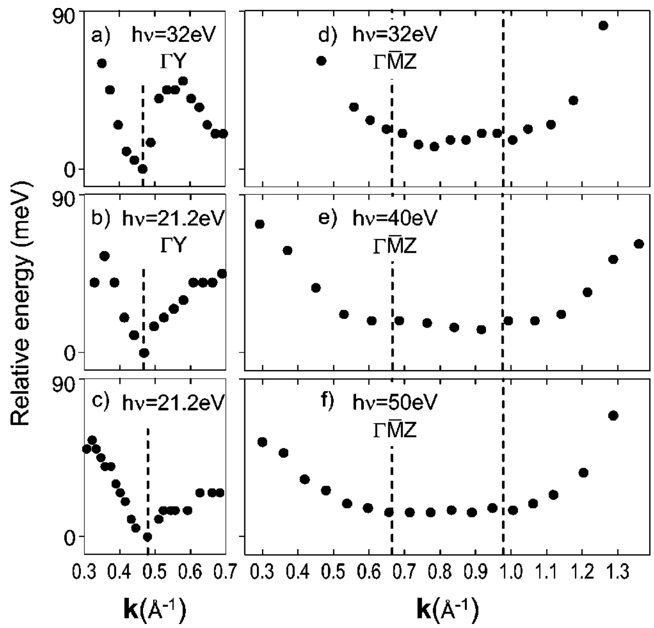

FIG. 3. Relative energy position of the leading edge of the ARPES spectra for: (a)–(c) the data shown in Fig. 2 in panels 1, 3, and 4, repectively; (d) the data shown in Fig. 2 in panel 2; (e) and (f) the data shown in Figs. 1(b) and (c), respectively. The dashed vertical lines mark the proposed position of $\mathbf{k}_F$. For (a)–(c) $\mathbf{k}_F$ is uncontroversial; for (d)–(f) the positions of $\mathbf{k}_F$ for the Γ-centered, electronlike FS proposed in Ref. 5 are indicated. Note that both the energy and the **k** scale are identical for (a)–(f).

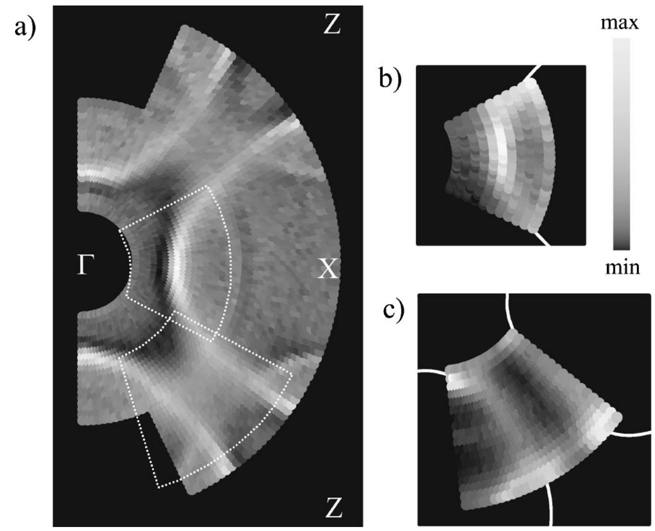

FIG. 4. FS maps of Bi-O modulation-free Pb-doped Bi2212 recorded using unpolarized radiation at room temperature. The grey scale indicates the photoemission intensity in a 20 meV window centered at E_F. (a) $h\nu=21.22$ eV (He I): The upper [lower] dotted areas indicate the portions of **k** space examined with $h\nu=40.8$ eV (He II) radiation in parts (b)[(c)] of the figure. The He I and He II FS maps were from consecutive cleavages of the same single crystal. Note the complete absence of any sign of a FS crossing along or near the $\Gamma\bar{M}$ line in (c).

plicit in the use of polarized synchrotron radiation (e.g., $h\nu=32$ eV). Furthermore, the DR features which decorate the ARPES data of pure Bi2212 make it harder still to find a suitable main FS crossing to use as a test system.

Therefore in order to determine the $I_{int}/I(E_F)$ signature of a main (right angular) FS crossing with dispersion equal to that seen along $\Gamma\bar{M}$ for $h\nu=32$ eV we turn to data from Pb-doped Bi2212, measured with unpolarized He I radiation ($h\nu=21.2$ eV). This approach has the following advantages: use of unpolarized radiation minimizes the differences in datasets recorded with different azimuthal angles and ARPES data from Pb-doped Bi2212 are simpler to interpret due to the absence of DR features.[12] In Fig. 2(b) we show the comparison between Pb-doped Bi2212 ARPES data for ΓY (panel 3) and for a different direction in **k** space [roughly from $0.4(\Gamma\bar{M})$ towards Y], representing a right-angular crossing of the main FS (panel 4). As is evident from Figs. 2(a) and (b), the dispersion relations of the bands in panels 2 and 4 are essentially identical—thus we have found a suitable candidate for our test. This search was only made possible by the use of the full-EDC FS map shown at the top of Fig. 2(b). The lower panels of Fig. 2(b) show without any doubt that the I_{int} and $I(E_F)$ characteristic of a main FS crossing is essentially unaffected by the steepness of the dispersion relation of the band coming up to the FS as *both* panels 3 and 4 of Fig. 2(b) show sharp peaks in $I(E_F)$ coupled to a steep drop in I_{int}. This, then, is in favor of our contention that the $h\nu=32$ eV $\Gamma\bar{M}$ data shown in Figs. 1 and 2(a) do not signal a main FS crossing in the Bi2212-based materials.

A further argument is based upon an analysis of the binding-energy position of the leading edge of the ARPES spectra. In our experience, based upon full-EDC FS maps comprising more than 4000 spectra,[10] the leading edge of the spectra not only approaches E_F as the band disperses up towards the FS, but also moves rapidly away from E_F again once the band has crossed the FS (this is a consequence of the well-known incoherent background present in ARPES data of all HTSC's). Thus, following the leading edge energy as a function of **k**, a main FS crossing exhibits a sharp dip centered at $\mathbf{k}_F$, as is illustrated in Fig. 3. Figures 3(a), (b), and (c) show analyses of the leading edge energy for the $h\nu=32$ eV data for ΓY [which is shown in panel 1 of Fig. 2(a)], and the He I data shown in Fig. 2(b) (panel 3) and Fig. 2(b) (panel 4), respectively. In all cases, the main FS crossing, and thus $\mathbf{k}_F$, are characterized by the sharp dip or ''V'' in the leading edge energy. This behavior is to be compared with that for the $\Gamma\bar{M}$ direction [Figs. 3(d)–(f)] in which, regardless of the photon energy, no sharp, V-like structure is seen in the leading edge energy profiles centered around the proposed FS crossing [$\mathbf{k}_F=0.81$ and 1.19 $(\Gamma\bar{M})$]. Thus it is clear that the leading edge data of Fig. 3(d) ($h\nu=32$ eV) should be grouped with the data of Figs. 3(e) and (f) which characterize flat-band, saddle-point behavior, and *not* with the leading edge datasets describing a main FS crossing [Figs. 3(a)–3(c)].

Taking the arguments given above, the viewpoint that the observed[5,6] FS ''crossings'' along the $\Gamma\bar{M}Z$ line in Bi2212 result, in fact, from the superposition of extrinsic DR features[10,13,14] is considerably strengthened. In Ref. 10 we argued that multiorder DR's combine to give a high intensity ribbon, visible in FS mapping data running along the $(0,-\pi)$-$(\pi,0)$ line. The suppression of the spectral weight from the extended saddle-point singularity states predicted for photon energies around 30 eV (Ref. 11), would then lead to a hollowing-out of the ribbon—leaving its edges intense enough to appear as a pair of FS crossings on either side of the $\bar{M}$ point. In order to test this point, and bearing in mind the efficacy of FS maps recorded using unpolarized radiation and based upon real, uninterpolated EDC's,[10] we have carried out such FS mapping experiments on Pb-doped Bi2212, in which the Pb substitution supresses the incommensurate Bi-O modulation[12] and thus switches off the DR features in the ARPES spectra.

Figure 4 shows the FS maps, in which $I(E_F)$ for a 20 meV energy window ($T=300$ K) is plotted. Data recorded using He I radiation ($h\nu=21.22$ eV) are shown in Fig. 4(a), whereas Figs. 4(b) and (c) contain smaller maps measured with He II ($h\nu=40.8$ eV) radiation which highlight those areas in **k** space indicated by the dotted lines in Fig. 4(a). In each case, the main holelike FS centered at the X and Y points is clearly visible (solid white line). While these conclusions are under no doubt for the He I data, upon consideration of Fig. 1, it can be seen that a photon energy of 40 eV is still in the critical range for which an intensity suppression near $\bar{M}$ is observed. Thus we point out that Fig. 4(c) ($h\nu=40.8$ eV) shows no indication of a FS crossing at the points 0.81 and 1.19 ($\Gamma\bar{M}$) as suggested in Ref. 5, nor at *any* point along or near to the $\Gamma\bar{M}Z$ line. Therefore the FS maps presented in Fig. 4, taken together with the detailed analysis of $I_{int}/I(E_F)$ (Fig. 2) and of the leading edge energies of the ARPES spectra (Fig. 3) offer very strong additional support to arguments that the alleged FS crossings along the $\Gamma\bar{M}Z$ direction in pristine Bi2212 are, in fact, due to DR features.[10,13] These dominate the ARPES spectra as a result of the matrix element-related supression of the saddle-point emission near $\bar{M}$ for photon energies around 30 eV.[11]

Thus, in summary, we can state that such DR-related ''FS crossings'' along $\Gamma\bar{M}Z$ in Bi2212 do not have any consequences for the true normal-state FS topology of the Bi2212-based HTSC's, which remains that of holelike barrels centered at the X,Y points, independent of the photon energy used in the ARPES experiment.

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[1] $X(Y)$ are the corners of the pseudotetragonal BZ, located at $2\pi/\mathbf{a}(\mathbf{b})\approx1.16$ Å^{-1}. $\bar{M}$ is the midpoint of XY in the two-dimensional BZ. We use the generally accepted shorthand: $\Gamma\equiv(0,0)$, $X\equiv(\pi,-\pi)$, $Y\equiv(\pi,\pi)$, $\bar{M}\equiv(\pi,0)$ and $Z\equiv(2\pi,0)$.

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