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Excitation energy dependence of the ARPES intensity in Pb-doped and pristine $Bi_2Sr_2CaCu_2O_{8+\delta}$

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Abstract

We report a systematic investigation of the photon energy ($h\nu = 18-29.5$ eV) dependence of the near-E_F photoemission intensity in Pb-doped and pristine $Bi_2Sr_2CaCu_2O_{8+\delta}$ high-temperature superconductors. We observe variations in the (π, 0)-spectra's line shape which are in good agreement with previous data and can be explained in terms of the different excitation probability (matrix elements) for each of the bilayer split bands. Moreover, we show that the photon energy dependence in the momentum distribution of the photocurrent at the Fermi level supports this interpretation. Similar trends in the momentum distribution maps of the pristine compound strongly suggest that the bilayer splitting is present also in near-optimally doped samples. A quantitative analysis of the (π, 0)-spectra in the superconducting state reveals a maximum of the bonding/antibonding ratio at $h\nu = 20-22$ eV. The photon energy dependence of the (π, π)-spectra, which are good representatives of the incoherent background, is also discussed.

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Understanding the electronic structure of complex materials requires information about their one-particle spectral function which can, at least in principle, be gathered by high-resolution angle-resolved photoemission spectroscopy (ARPES). However, matrix elements can play a crucial role

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in the photoemission process and their influence on the spectra has to be studied carefully in order to extract the desired information. As shown recently for high-T_c superconducting (HTSC) cuprates [1–5], the photon energy is the experimental parameter with the largest influence on the matrix elements. For $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi2212) the proximity of two CuO-layers gives rise to a splitting of the conduction band and it turns out that the matrix elements can be substantially different for these split bands. Thus, the spectra are sometimes dominated by one of the bands, almost completely masking the presence of the other.

This has important consequences. In a previous study of Bi2212 [3,5] we have shown that the line shape of the spectra recorded at the $(\pi, 0)$-point in the modulation-free Pb-Bi2212 is strongly excitation energy dependent and such dependence as well as the lineshape itself were interpreted, with some exceptions, to be the result of the bilayer splitting. There are, however, still open issues which can question this interpretation. One can argue, for instance, that the varying angle of incidence required by the geometry of the experiment could be responsible for the observed changes or that the background, approximated by a universal empirical line shape, can turn out to be photon energy dependent. Finally, the most convenient photon energy region for ARPES experiments, 15–30 eV, was covered only with 6 points. Still another question concerns the validity of the same conclusions regarding pristine Bi2212. If in overdoped case it seems to be well established, it was suggested recently [6] that in the optimally doped samples no evidence for a bilayer splitting can be found. Since the $(\pi, 0)$-region is, in terms of ARPES spectral weight, the most sensitive to the onset of superconductivity, it is desirable to further compile information which helps to understand in detail which portion of complexity in the line shape comes from the bilayer splitting and what is the result of the many body effects possibly related to the superconductivity itself.

In this Report we confirm our previous interpretation [3,5] using a different apparatus and experimental geometry. Most importantly, and unlike in most other systems, the emission angle of the electrons relative to the surface is changed by moving the electron analyzer and not the sample, leaving the angle between sample and incident light constant. We show that the $(\pi, 0)$-spectra in the superconducting state depend on the photon energy and that the variations of their line shape can indeed be explained in terms of the bilayer splitting. Moreover, a detailed study of the photon energy dependence of the $(\pi, 0)$- and (π, π)-spectra reveals that the bonding/antibonding spectral weight ratio is a smoothly varying function of the excitation photon energy with the local maximum near 20–22 eV, which agrees well with our previous results. Momentum distribution maps recorded as a function of photon energy for Pb-Bi2212 and pure Bi2212 samples show similar trends in intensity variations implying the presence of bilayer splitting also in the optimally doped Bi2212.

The photoemission experiment was performed using an angle-resolved electron spectrometer at the SGM-3 beamline on the undulator of the storage ring ASTRID in Aarhus. A detailed description of the instrument will be given elsewhere [7]. In short, the beamline covers an energy range from 12 eV to 140 eV with a resolving power better than 15000. For the measurements reported here, the light was incident under an angle of 50° away from the surface normal. The light was linearly polarized and all the plots of Fermi level scans in this paper are oriented such that the polarization direction of the light is horizontal. The electron spectrometer is a commercial VG ARUPS 10 analyser which is mounted on a goniometer inside the chamber and equipped with a multichannel detector. The analyser position can be changed by motors outside the chamber. The total energy resolution used in this work was 130 meV for Fermi level scans and 28 meV for the lineshape analysis. The angular resolution was around ±0.7°. The sample temperature was around 30 K. The pressure during the experiments was in the mid 10^{-11} mbar range. High quality single crystals of the overdoped Pb-Bi2212 ($T_c = 69$ K) and near-optimally doped Bi2212 ($T_c = 89$ K) were cleaved in situ to provide mirror like surfaces.

In Fig. 1 we show spectra recorded in $(\pi, 0)$- and (π, π)-points of the Brillouin zone (BZ) as well as

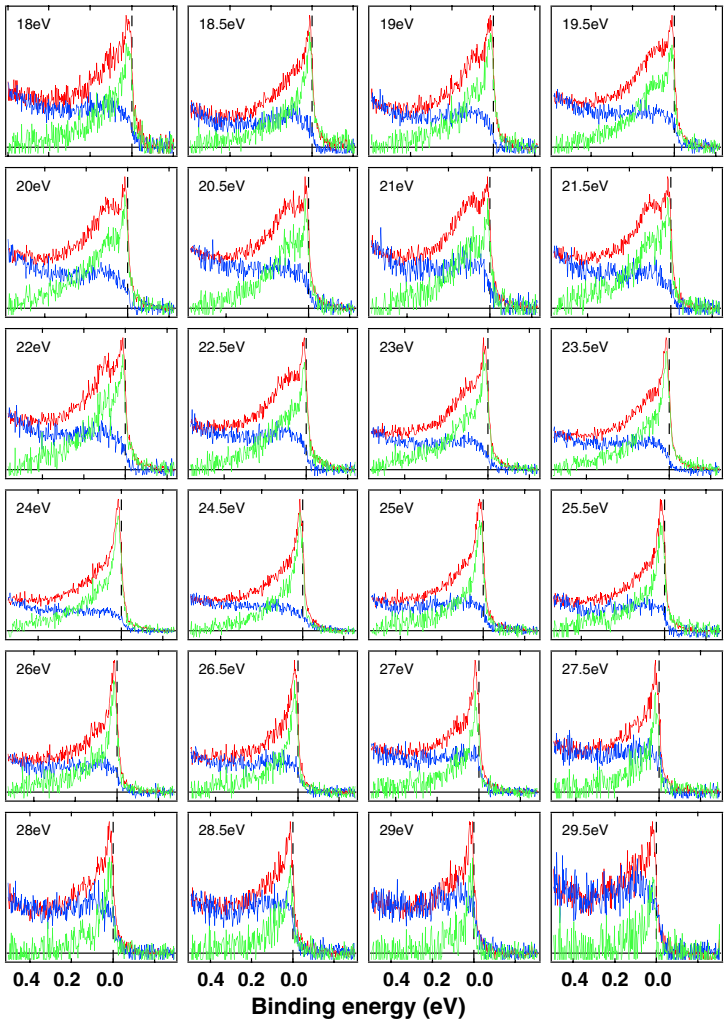

Fig. 1. The (π, 0) [red] and (π, π) [blue] photoemission spectra from the Pb-Bi2212 sample together with their difference [green], representing the superposition of the bonding and antibonding bands. For interpretation of the reference in color in this figure legend, the reader is referred to the web version of this article.

their difference as a function of the excitation photon energy. Spectra are brought into the same intensity scale by normalizing them to the intensity at a binding energy of 500 meV. As in the previous study [3], it is seen that the (π, 0)-spectra are sensitive to the photon energy. What is new here is that the difference spectra are also energy dependent. This means that the line shape variations of the (π, 0)-spectra cannot be explained by the energy dependent background. As Fig. 1 shows, our empirical approximation of the background line shape used in Ref. [3] is justified.

Before we discuss this dependence in details it is worth to briefly address the question of the background. The reason why we subtract exactly the (π, π)-spectrum is the following. We believe that it is the most suitable representative of the incoherent spectral weight, which is widely accepted to be **k**-independent and routinely observed in the ARPES spectra of HTSC cuprates since long ago. It is the (π, π)-point of the BZ which corresponds to the unoccupied part and where one does not expect any influence of additional features, like shadow bands or diffraction replicas [8]. As seen

from the matching behaviors in the higher binding energy part of the spectra this choice of the background is quite successful. As for the background line shape itself, as follows from Fig. 1 its variations with photon energy are rather insignificant. Since at the same time the changes of the (π, 0)-spectra are apparent, this observation supports the idea that the background should be considered as something extrinsic rather than a part of the spectral function.

Already a visual inspection of the difference spectra shown in Fig. 1 allows to notice the enhancement of the "hump" feature located at ~90 meV when using the 20–22 eV photon energies. In spite of the different experimental geometry and a different procedure of the background subtraction this is in agreement with the data reported in Ref. [3]. As a step towards a quantitative analysis we apply here the same two-peak fitting procedure as in Ref. [3]. We do not consider here the "third" feature since its spectral weight is expected to be very small for the overdoped samples and photon energy range in question (18–29.5 eV). The typical result of the fit is shown in Fig. 2(a). For each of the two features we use identical spectral functions of the type:

$$A(\omega,\varepsilon,T)\propto\frac{|\,\Sigma''(\omega,T)\,|}{(\omega-\varepsilon)^2+\Sigma''(\omega,T)^2}, \tag{1}$$

where $\Sigma''(\omega,T)=\sqrt{(\alpha\omega)^2+(\beta T)^2}$ is the renormalized [3] imaginary part of the self-energy with $\alpha=1$, $\beta=2$ and the temperature T is in energy units. Such a choice of the self-energy was found to be the most successful and approximately corresponds to the Marginal Fermi Liquid approach. Thus, for the fitting function we have:

$$I(\omega,T,h\nu)\propto[(M_a(h\nu)A(\omega,\varepsilon_a,T)+M_b(h\nu)A(\omega,\varepsilon_b,T))f(\omega,T)]\otimes R_\omega, \tag{2}$$

where $f(\omega,T)$ is the Fermi function and R_ω is the Gaussian with the 28 meV full width at the half-maximum. The components of the spectrum are shown in Fig. 2(a) as area plots: light and dark grey colors represent the bonding and antibonding bilayer bands, respectively. We get the best quality of the fit when the positions of the features are:

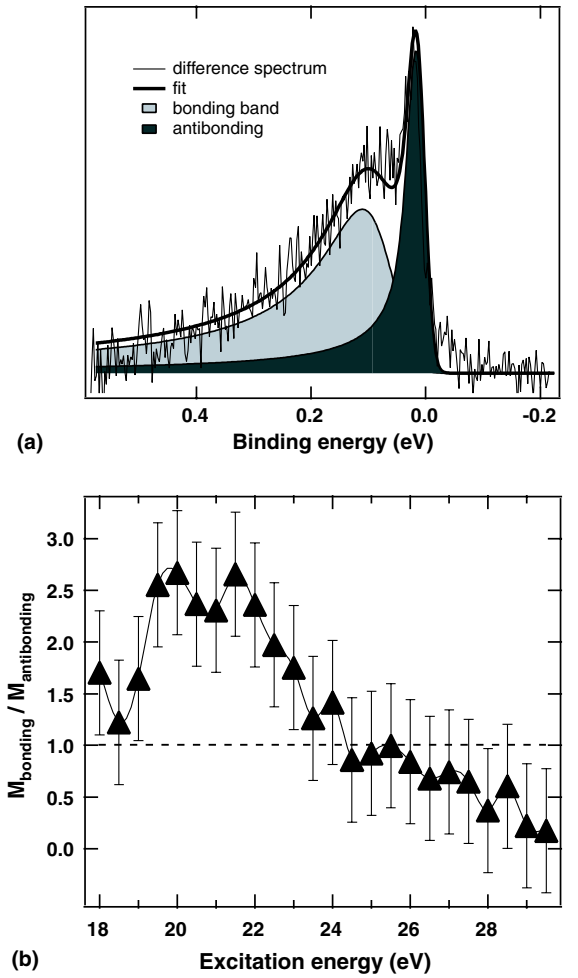

Fig. 2. (a) Exemplary fit of the difference spectrum and its bonding and antibonding components at $h\nu=20$ eV. (b) The ratio M_b/M_a as a function of photon energy.

$\varepsilon_a=11(3)$ meV and $\varepsilon_b=154(6)$ meV, giving a value of ~140 meV for the bilayer splitting in the (π, 0)-point.

In Fig. 2(b) we show the ratio of the fit parameters M_a and M_b representing the matrix elements as a function of photon energy. The obtained curve is in good qualitative and even quantitative correspondence with the data reported before. The more detailed energy dependence provides an important argument in favor of the matrix elements scenario—both prefactors are smoothly varying functions, as expected in accordance with the theoretical calculations [9]. The existence of the

maximum near 20–22 eV has a big practical meaning because it opens a possibility to study nearly independently one of the split components [4]. It also partially explains why the bilayer splitting has escaped the attention of many ARPES groups for so long. The nearly 2.5 times stronger emission from the bonding band will mask the presence of the antibonding component at higher temperatures and/or moderate momentum resolution when using the popular laboratory-based He-lamp radiation of 21.2 eV.

To further check the suggested interpretation we have extended our study to a larger part of the Brillouin zone by measuring the momentum distribution at the Fermi level using different excitation energies. Such momentum distributions, also known as a "Fermi-surface maps" when taken in the normal state, were already shown to be strongly photon energy dependent [10–12,1,13,14]. Again, only a few photon energies were used in the energy range of 18–30 eV investigated here. Moreover, if the light is linearly polarized, the momentum distribution of the intensity also depends dramatically on the geometry [14]. Therefore we have chosen here the geometry of the experiment in such a way that apparently unfavorable conditions for the emission from particular states are avoided.

In Fig. 3 we show the results of the comparative study of Pb-Bi2212 and pristine Bi2212 samples. In agreement with the "matrix elements plus bilayer splitting" scenario, the presented maps are sensitive to the photon energy. In spite of the presence of the additional features like shadow Fermi surfaces in the case of Pb-Bi2212 and additionally diffraction replica in the pure Bi2212 [8], one can identify the spectral weight transfer from the bonding band to the antibonding one when going from 20 eV to 29 eV. One can observe a smooth transition from a hole-like Fermi surface to what appears to be an electron-like Fermi surface. This is exactly what is expected according to Fig. 2(b). We note, however, that the fitting results (see Fig. 2a) always indicate that the antibonding band is very close but still located *below* the Fermi level in the $(\pi, 0)$-point, even for the overdoped samples, thus implying that the antibonding sheet of the Fermi surface is topologically similar to the bonding one, i.e. it is hole-like.

An important observation here is that the trend in the redistribution of the intensity in the maps is the same for both Pb-Bi2212 and Bi2212 compounds. This strongly suggests that the reason for such an evolution in the optimally doped Bi2212 must have a similar origin as in the overdoped Pb-doped samples. Our results thus indicate the presence of bilayer splitting in optimally doped pristine Bi2212, which is in agreement with Ref. [1]. This conclusion is somewhat contradictory to recent claims as for the absence of the bilayer

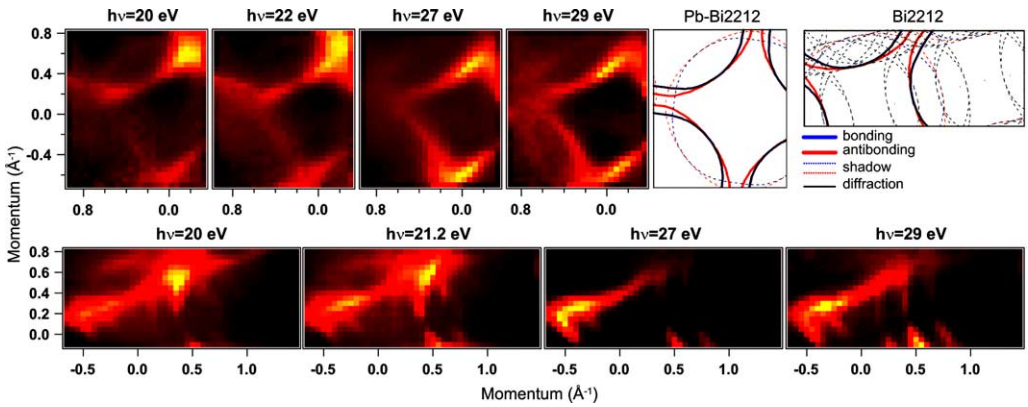

Fig. 3. Momentum distribution maps at E_F taken at ~30 K for Pb-Bi2212 (upper panel) and pure Bi2212 (lower panel). The sampled portions of the k-space together with a sketch of the expected Fermi surface segments is shown on the upper panel to the right.

splitting in Bi2212 made in Ref. [6], although the superconducting state was not a subject of the debates there.

In conclusion, for the bilayer Bi2212 systems we have shown that the interpretation of the peak-dip-hump line shape of the superconducting state (π, 0)-spectra in terms of a superposition of the bonding and antibonding bands given in Ref. [3] is valid, as confirmed by systematic measurements using considerably different experimental conditions. Within the 18–29.5 eV energy range, the ratio of the bonding and antibonding spectral contributions is found to be a smoothly varying function of the photon energy which has the local maximum at ~20–22 eV. The momentum distribution of the photoemission intensity at the Fermi level turns also out to be sensitive towards the photon energy and supports the conclusions drawn from the (π, 0)-spectra line shape analysis. Similar trends in the momentum distribution maps of pure Bi2212 suggest the presence of bilayer splitting in this nearly optimally doped compound. Moreover, we show that the (π, π)-spectra do not exhibit a strong energy dependence and are good representatives of the incoherent background.

Acknowledgments

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