V. D. Borysenko, Cand. Sc. (Eng.), Assist. Prof.; V. H. Borysenko

RESEARCH OF THE ELECTRONIC STRUCTURE AND ELECTRONIC PROPERTIES OF THE METALLIC MONOLAYER ON THE SURFACE OF THE HIGH-TEMPERATURE SUPERCONDUCTOR BY ANGLE-RESOLVED PHOTOEMISSION SPECTROSCOPY (REWIEV OF EXPERIMENTAL PAPERS)

By means of angle-resolved photoemission spectroscopy (ARPES) there had been carried out the detailed comparative study of the series of YBCO samples with different charge carrier concentration (from 0.05 to 0.25 holes per unit cell) doped by oxygen and calcium is carried out. It is shown that the photoemission spectrum, as a rule, consists of two components: metallic and superconducting, which represent the signals from the first surface CuO_2 bilayer and bulk. By the analysis of the spectra received these bulk and surface signals are separated and peculiarities of their electronic properties are researched.

***Key words**: photoemission spectroscopy, high – tc superconductor, surface signals.*

Introduction

Photoemission spectroscopy has a very important influence on the modern researches of the electronic structure of solids. With aid the of angular resolution it is possible to obtain the information about the topology of the Fermi surface, quasiparticle dispersion, magnitude and momentum distribution of the energy gaps etc. Photoemission spectroscopy is widely applied to study the high-temperature superconductors, in which the mechanism of superconductivity remains unexplained. With aid of ARPES the anisotropy of the superconducting energy gaps had been established, the dominant factors influencing the quasiparticle dynamics had been determined, the Fermi surface had been studied in details. The vast majority of investigations has been carried out on the so-called BSCCO cuprates, whereas not less famous YBCO compounds remained nearly unexplored because of the considerable contribution of the surface states to the photoemission signal. Thus, there is a necessity in separating the surface and bulk photoemission signal in YBCO compounds.

Experiment

The data had been obtained using the standard photoelectron spectrometer with angular resolution SCIENTA SES 100 and high intensity sources of synchrotron radiation BESSY (Germany) and SLS (Switzerland) [1,2]. Samples have been mounted on the cryo-manipulator. Atomically clean surface had been obtained in ultra-high vacuum of the order of $5\ 10^{-11}$ mBar by mechanical cleavage of the samples along the crystalographic surfaces. All spectra had been recorded with the energy resolution of 12 meV and angular resolution 0.2°. Fermi level has been calibrated using the Fermi edge of the polycrystalline silver film evaporated on the surface of the manipulator along with the studied sample. High quality single crystals of YBCO have been synthesized by growth from melt and oxyginated to the necessary level. The crystal structure of YBCO is shown in Fig.1. Here we show the data collected from two samples $YBa_2Cu_3O_{6.85}$ with T_C = 90 K and $YBa_2Cu_3O_{6.4}$ with T_C = 35 K, which were untwinned by the mechanical stress at rising temperature. A couple of twinned crystals have also been studied: $YBa_2Cu_3O_{6.9}$ and $Y_{1-x}Ca_xBaCu_3O_{7-d}$, with x = 0.15 and with T_C = 90 and 77 K, correspondingly.

Experimental results

Electronic structure of the untwinned $YBa_2Cu_3O_{6.85}$ with T_C = 90 K is shown in Fig.2. The upper panel contains two experimental Fermi surface maps (color scale) measured along Γ-X and Γ-Y directions as well as the model electronic structure in the tight-binding approximationi in panels (a)–(d) the photoemission spectra along the different directions of the Brillouin zone indexed above by the corresponding letters are shown. Similarly, the data for $YBa_2Cu_3O_{6.4}$ with T_C = 35 K are given in Fig. 3. In contrast to the previous photoemission studies of YBCO [3-6], the higher photon energies have been used (50–60 eV in comparison with 15–30 eV), which allowed to significantly increase the intensity of the photoelectrons and cover larger areas in the momentum space.

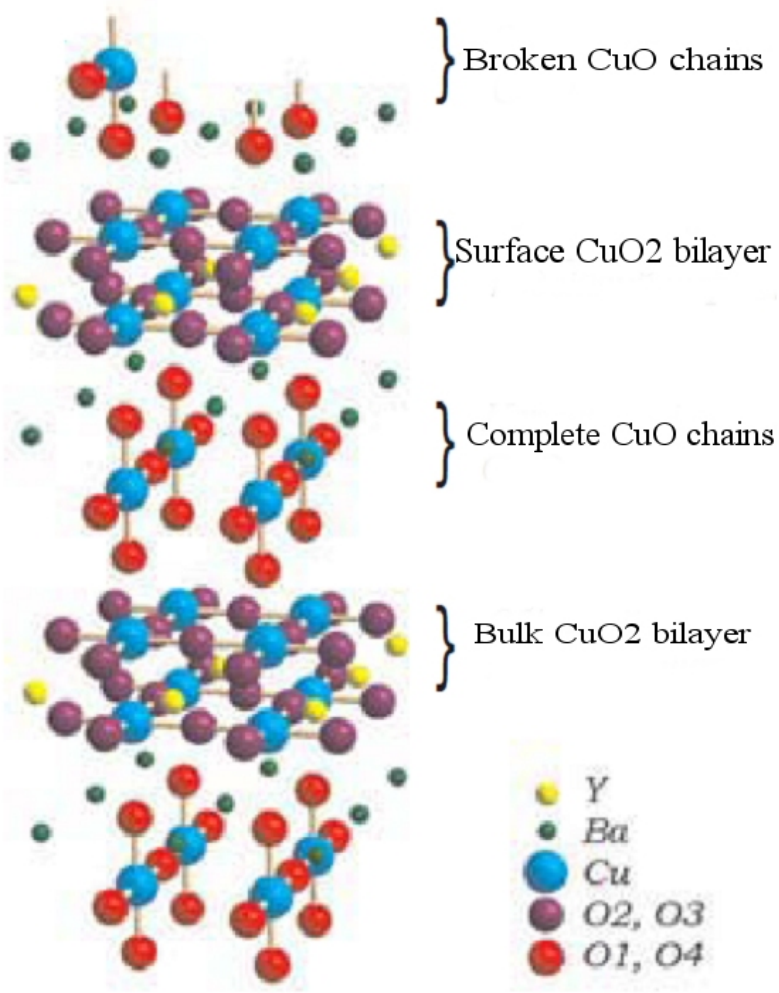


Fig. 1. Crystal structure of YBa2Cu3O7−d.

Visually, the correspondence between the experimental and calculated [7] electronic structure appears to be a complete one. There are two hole-like Fermi surfaces around S-points.

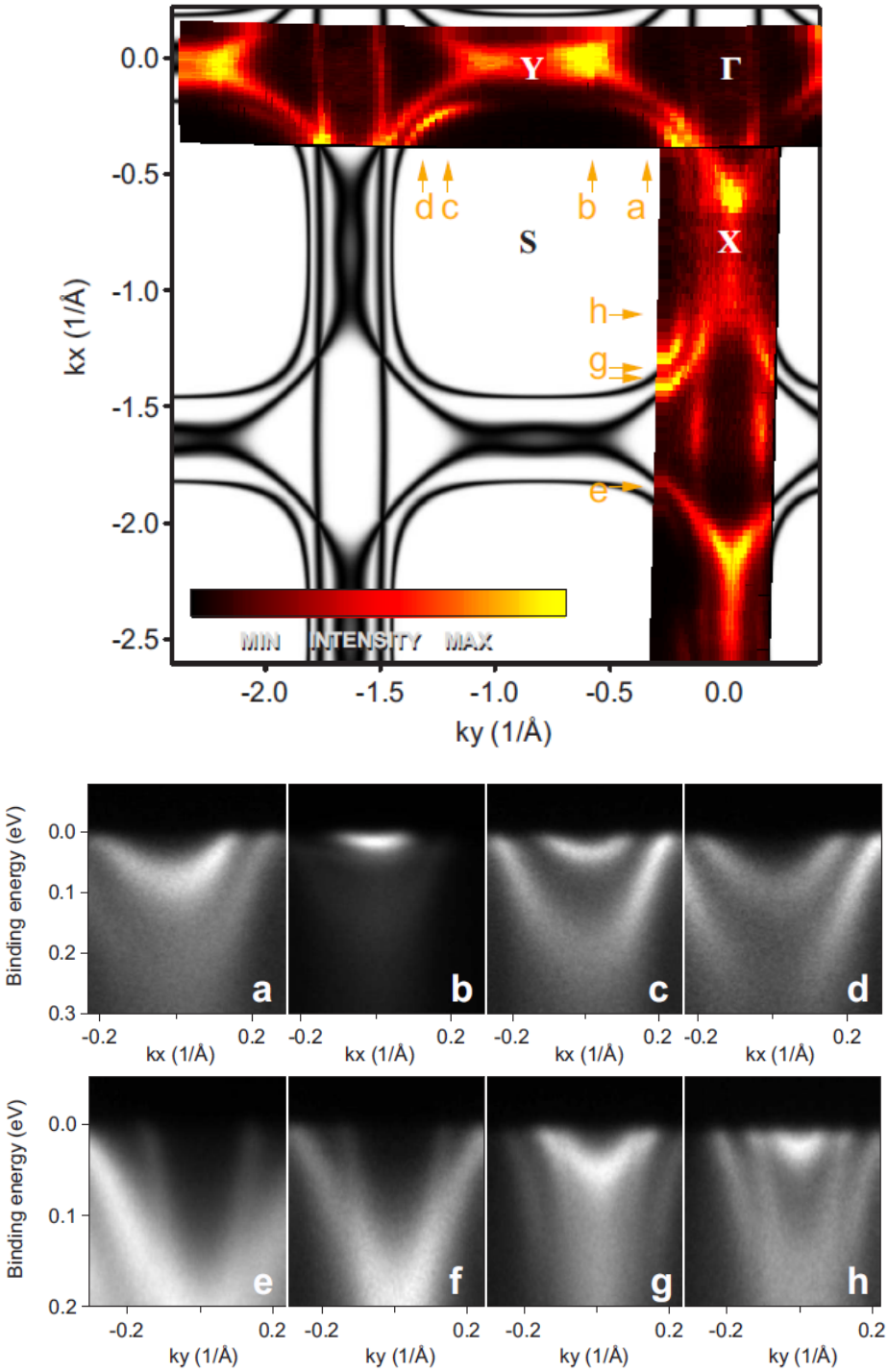


Fig. 2. Experimental electronic structure of the untwinned $YBa_2Cu_3O_{6.85}$, $T_C = 90$ K

Upper panel contains two experimental Fermi surface maps (color scale) measured along Γ-X and Γ-Y directions and modelled electronic structure in the tight-binding approximation. a–h – photoemission spectra in different directions of the Brillouin zone, designated by the letters above.

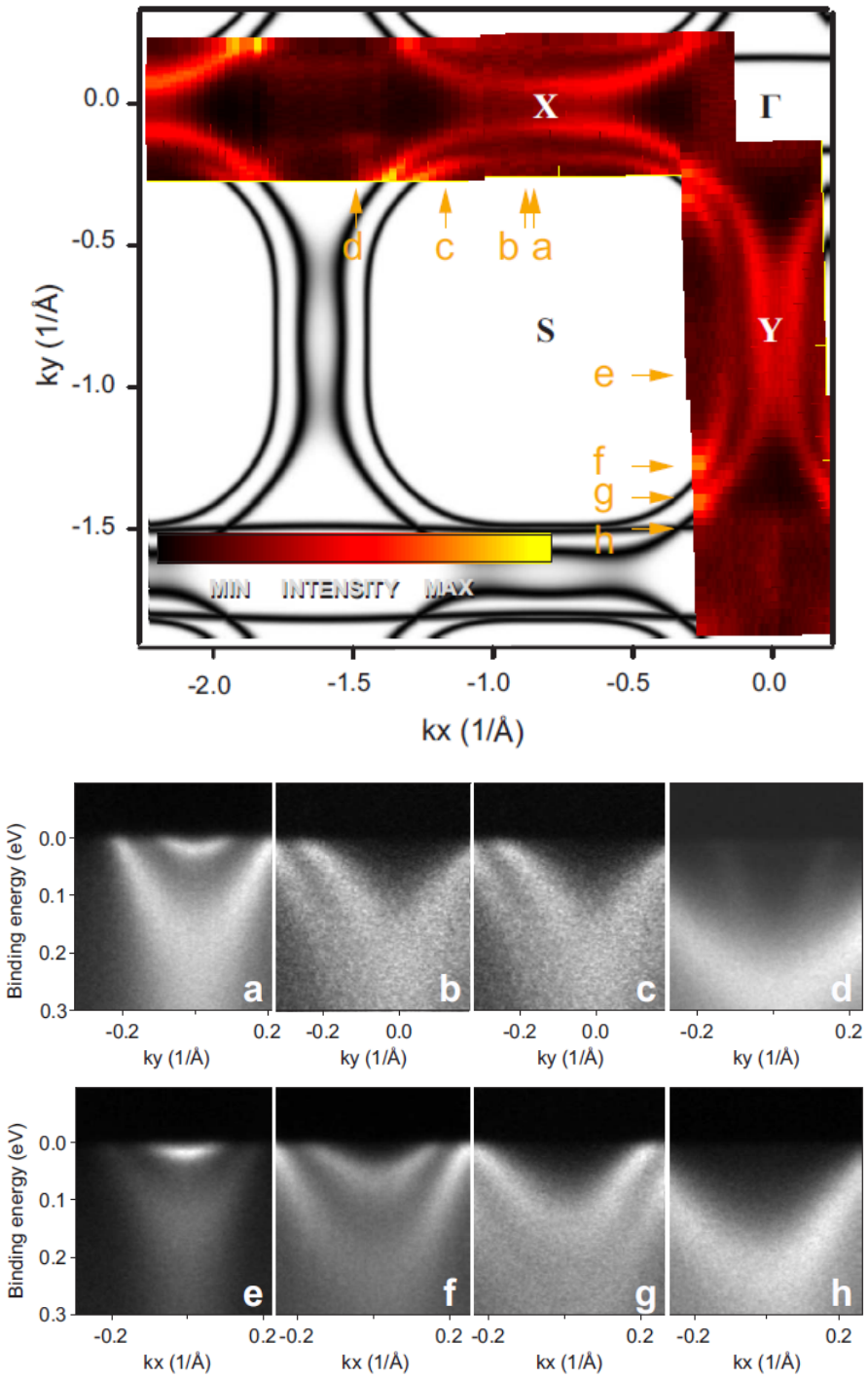


Fig. 3. As in Fig.2, experimental electronic structure of the untwinned $YBa_2Cu_3O_{6.4}$, $T_C = 35$ K

All data are collected with T = 30 K. (b)-(h) panels had been measured using the photons of hv = 50 eV and linear polarization, (a) spectrum had been obtained using the photons of hv = 55 eV.

One-dimensional structure along Γ-X direction is a direct evidence of the existence of the electronic states related to CuO chains. It is also interesting that, unlike in $Bi_2Sr_2CaCu_2O_{8+d}$ [8], the splitting of the conduction band due to the presence of two neighboring CuO_2 layers is more isotropic. Thus, one can draw a conclusion that on the qualitative level, the full correspondence

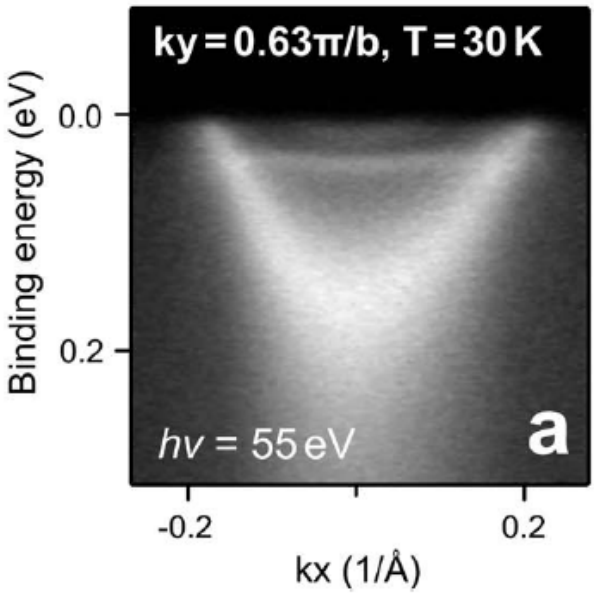
between the experimental electronic structure of YBCO and LDA calculations [7] is found.

However, on the quantitative level there is a substantial difference. Namely, the charge carrier concentration (in this case holes), which is proportional to the area of the Fermi surface [9], is equal to 0.31. This considerably exceeds the value x = 0.15, which is expected for the sample with T_C = 90 K. Besides, the expected modification of the electronic structure (opening of the superconducting gap) when going below T_c is not observed. Further researches also disclosed an unusual structure, which appears in the spectra at low temperatures. In Fig. 4a this structure is seen as a band with the weak dispersion at energies of approximately 40 meV.

Fig. 4b explains this "unusual" structure as strongly renormalized band, which is a consequence of both, opening of the superconducting gap and interaction with the famous magnetic resonance [10]. Experimental spectrum shown in Fig. 4a is thus a superposition of signals from the superconducting (bulk) and metallic (surface) components. The lowest panel in Fig. 4B represents the superconducting spectrum, the middle one — the metallic and the top one — their superposition.

The origin of such two-component spectrum becomes clear if one considers the crystal structure of YBCO (Fig. 1), which is also shown schematically in Fig. 4c. Photoemission signal is the superposition of the signal from the first surface bilayer CuO_2 and weaker signal form the bulk of the sample. The doping level of the closest to the surface bilayer CuO_2 is changed because of the broken chains CuO on the surface which act as a charge reservoir in these compounds. The chains which are left intact on the surface increase the hole concentration in the surface layer CuO_2, whereas the broken ones decrease it. With this, the regions with the reduced holes concentration acquire the properties of the Mott-insulator and do not contribute to the quasiparticle spectrum at the Fermi surface. Thus, the most intense is the signal from the most overdoped (x = 0.31), and correspondingly non-superconducting, near-surface bilayer CuO_2, and the other component of the spectrum originates from the bulk of the sample with the nominal doping level.

The temperature dependence of the mentioned above "unusual" structure shown in Fig. 5 confirms this interpretation and fully corresponds to the temperature evolution of the analogous spectrum in BSCCO [10]. By changing the chemical composition of the crystal, for example by Ca substitution, it is possible to achieve the full suppression of the surface-related signal (see Fig. 6).



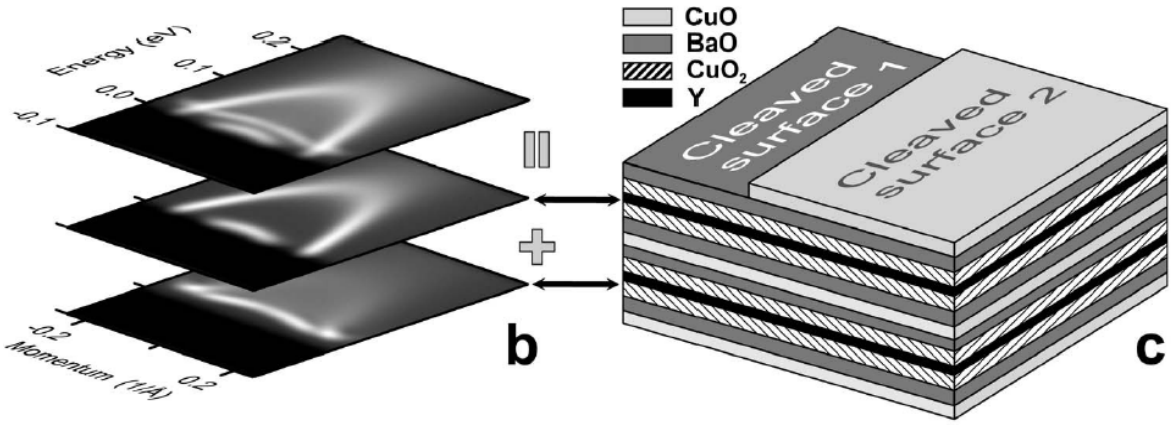
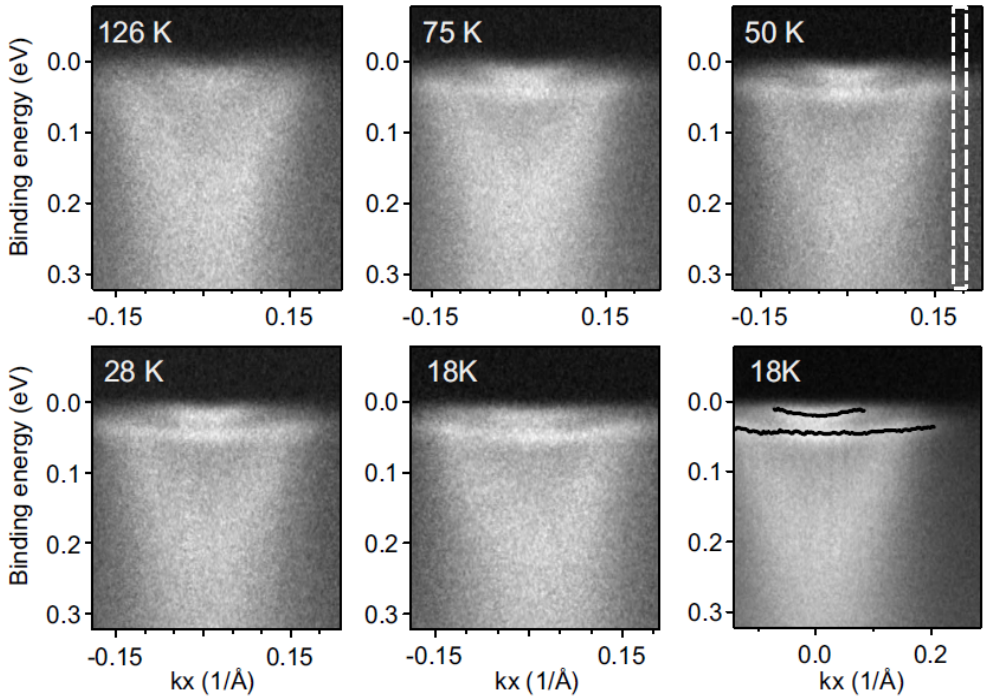


Fig. 4. Coexistence of the metallic and superconducting components of the photoemission spectrum. (a) Experimental spectrum which consists of the contributions of the metallic and superconducting components for YBa2Cu3O6.85, ky = 0.63 □/b, T = 30 K, hv =55 eV. (b). Schematical illustration explaining the experimental spectrum as a superposition of the signals from the superconducting (bulk) and metallic (surface) components. The lowest panel represents the superconducting spectrum, the middle one — metallic and the topmost one — their superposition. (c) Schematic illustration of the single crystal surface of YBCO. The doping level of the closest to the surface CuO2 bilayer is changed as a consequence of the broken CuO chains at the surface which act as a charge reservoir in these compounds.



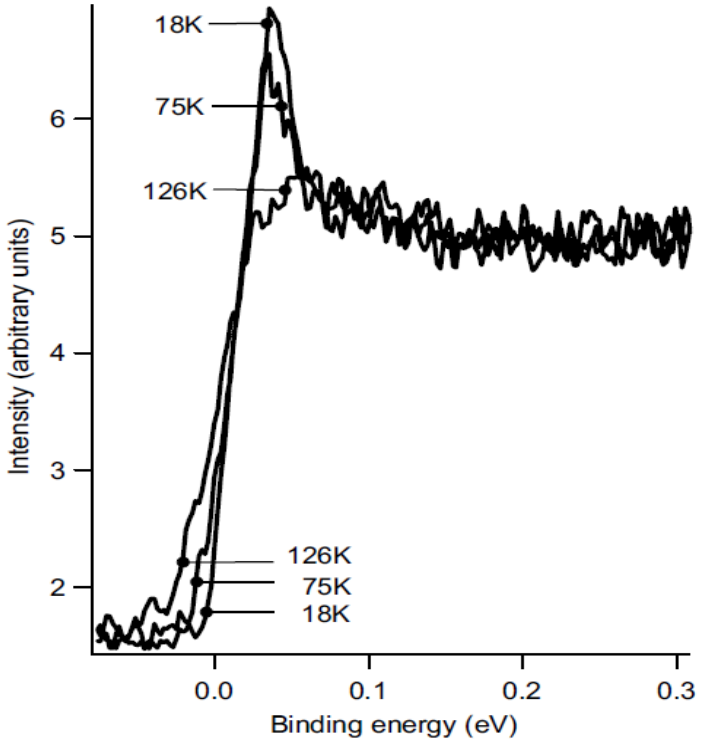
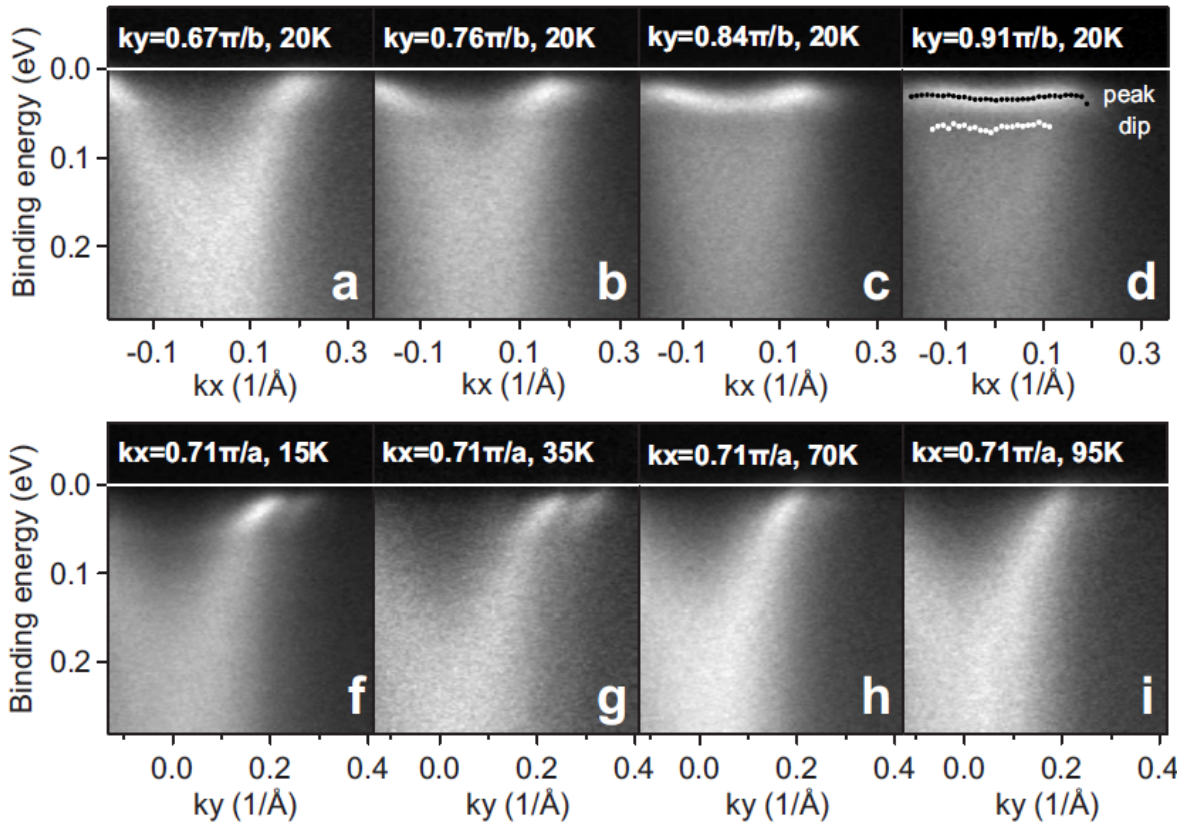


Fig. 5. Temperature dependence of the superconducting component for $YBa_2Cu_3O_{6.9}$.
Lower panel contains the energy distribution curves (EDC) integrated within the narrow momentum range shown in panel “50 K”.



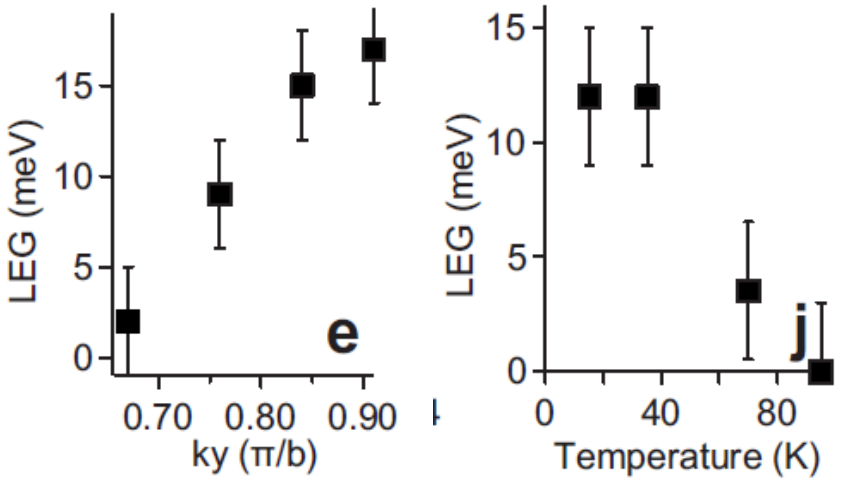


Fig. 6. Superconducting component in $Y_{1-x}Ca_xBaCu_3O_{7-d}$, with x = 0.15 and with T_C = 77 K. (a)-(d): Opening of the superconducting gap and increase of the renormalization upon approaching the antinodal region. (f)-(i): Evolution of the spectrum with the increase of the temperature.

Conclusions

1. Photoemission spectra of $YBa_2Cu_3O_{7-d}$ consist, as a rule, of two components: metallic and superconducting ones, which represent the signals from the first near-surface CuO_2 bilayer and from the bulk of the sample respectively.
2. The near-surface CuO_2 bilayer turns out to be overdoped with the concentration of the carriers of about 0.3 holes per unit cell, which is nearly independent from the stoichiometry of the bulk of the sample.
3. The quasiparticle spectrum is renormalized by the opening of the superconducting gap with d-wave symmetry in the bulk of the YBCO-samples in the superconducting state.
4. As in the case of $Bi_2Sr_2CaCu_2O_{8+d}$, elecronic structure in the bulk of YBCO reveals strongly anisotropic renormalization, which is maximal in the antinodal regions and disappears above Tc. This supports the universality of the conclusion as for the magnetic origin of the anisotropic renormalization in HTSC.

REFERNCES

1. V Zabolotnyy V. B. Momentum and temperature dependence of renormalization effects in the high-temperature superconductor Yba2Cu3O7?d / V. B. Zabolotnyy, S. V. Borisenko, A. A. Kordyuk et al. // Phys. Rev. – 2007. – B 76. – P. 064519 (1 – 5).

2. Kordyuk A. A. Constituents of the quasiparticle spectrum along the nodal direction of high-Tc cuprates / A. A. Kordyuk, S. V. Borisenko, V. B. Zabolotnyy et al. // Phys. Rev. – 2006. – Lett. 97. – P. 017002 (1 – 4).

3. Gofron K. Occurrence of van Hove singularities in YBa2Cu4O8 and YBa2Cu3O6.9 / K. Gofron, J. C. Campuzano, H. Ding et al. // J. Phys. – 1993. – Chem. Solids. 54. – P. 1193 – 1198.

4. Schabel M. C. Angle-resolved photoemission on untwinned YBa2Cu3O6.95. I. Electronic structure and dispersion relations of surface and bulk bands / M. C. Schabel, C.-H. Park, A. Matsuura, Z.-X. Shen, D. A. Bonn // Phys. Rev. – 1998. – B 57. – P. 6090 (1 – 4).

5. Schabel M. C. Angle-resolved photoemission on untwinned YBa2Cu3O6.95. II. Determination of Fermi surfaces / M. C. Schabel, C.-H. Park, A. Matsuura, Z.-X. Shen, D. A. Bonn, Ruixing Liang, and W. N. Hardy // Phys. Rev – 1998. – B 57. – P. 6107 (1 – 6).

6. Lu D. H. Superconducting Gap and Strong In-Plane Anisotropy in Untwinned Yba2Cu3O7-d / D. H. Lu, D. L. Feng, N. P. Armitage, K. M. Shen, A. Damascelli, C. Kim, F. Ronning, Z.-X. Shen, D. A. Bonn, R. Liang, W. N. Hardy, A. I. Rykov, and S. Tajima // Phys. Rev. – 2001. – Lett. 86. – P. 4370 (1 – 5).

7. Andersen O. K. LDA energy bands, low-energy hamiltonians, t', t_p, t (k), and J / O. K. Andersen, A. I. Lichtenstein, O. Jepsen, and F. Paulsen // J. Phys. – 1995. – Chem. Solids. 56. – P. 1573 – 1578.

8. Kordyuk A. A. Evidence for CuO conducting band splitting in the nodal direction of Bi2Sr2CaCu2O8+d / A. A. Kordyuk, S. V. Borisenko, A. N. Yaresko et al. // Phys. Rev. – 2004. – B. 70. – P. 214525 (1 – 5).

9. Luttinger J. M. Fermi Surface and Some Simple Equilibrium Properties of a System of Interacting Fermions / J. M. Luttinger // Phys. Rev. – 1960. – 119. – P. 1153 (1 – 4).

10. Borisenko S. V. Anomalous Enhancement of the Coupling to the Magnetic Resonance Mode in Underdoped Pb-Bi2212 / S. V. Borisenko, A. A. Kordyuk, T. K. Kim, A. Koitzsch, M. Knupfer, M. S. Golden, J. Fink, M. Eschrig, H. Berger, and R. Follath // Phys. Rev. – 2003. – Lett. 90. – P. 207001 (1 – 6).

Volodymyr Borysenko – Cand. Sc. (Eng), Assistant Professor with the Department of Physics and Photonics, e-mail: vdbor@svitonline.com.

Vinnytsia National Technical University.

Viktorija Borysenko – Master.

Vadym Hetman Kyiv National Economic University.