Physica C 469 (2009) 448–451

Contents lists available at ScienceDirect

Physica C

journal homepage: www.elsevier.com/locate/physc

Fermi surface of $Ba_{1-x}K_xFe_2As_2$ as probed by angle-resolved photoemission

V.B. Zabolotnyy [a,*], D.V. Evtushinsky [a], A.A. Kordyuk [a,b], D.S. Inosov [c], A. Koitzsch [a], A.V. Boris [c,d], G.L. Sun [c], C.T. Lin [c], M. Knupfer [a], B. Büchner [a], A. Varykhalov [e], R. Follath [e], S.V. Borisenko [a]

[a] Leibniz Institute for Solid State and Materials Research, IFW-Dresden, P.O. Box 270116, D-01171 Dresden, Germany
[b] Institute of Metal Physics of National Academy of Sciences of Ukraine, 03142 Kyiv, Ukraine
[c] Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany
[d] Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom
[e] Elektronenspeicherring BESSY II, Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Strasse 15, 12489 Berlin, Germany

ARTICLE INFO

Article history:
Available online 19 March 2009

PACS:
74.25.Jb
74.70.−b
79.60.−i

Keywords:
Pnictides
Fermi surface
ARPES
Superconductivity

ABSTRACT

Here we apply high resolution angle-resolved photoemission spectroscopy (ARPES) using a wide excitation energy range to probe the electronic structure and the Fermi surface topology of the $Ba_{1-x}K_xFe_2As_2$ (T_c = 32 K) superconductor. We find significant deviations in the low energy band structure from that predicted in calculations. A set of Fermi surface sheets with unexpected topology is detected at the Brillouin zone boundary. At the *X*-symmetry point the Fermi surface is formed by a shallow electron-like pocket surrounded by four hole-like pockets elongated in $\Gamma-X$ and $\Gamma-Y$ directions.

Since the discovery of superconductivity in Fe-based pnictides [1,2] with critical temperatures comparable to those of the famous layered cuprate high-T_c superconductors [3–8], the interest raised by these materials seems to excel the one evoked by the discovery of cuprates. Important conclusions as for the nature of the superconductivity [9], symmetry of the superconducting order parameter [10–12] and its absolute value [13–15] are currently being made, while the electronic structure of the novel type of superconductors remains controversial. According to early angle-resolved photoemission studies (ARPES) [14,16–18], the band structure calculations [17,19–23] seem to capture the most essential ingredients of the low-lying electronic structure. The basic result of the band structure calculations is that the inequivalence of the As sites in the "parent" compound $BaFe_2As_2$ (BFA) results in a Fermi surface (FS) folding into two concentric hole-like FS sheets centered at the Γ-point and double-walled electron-like pockets at the *X* and *Y* points. In another *parent* Fe-based system LaOFeP even more remarkable agreement was found [24]. However, in the case of *doped* superconducting BKFA the experimental reports concerning the FS topology are far from been equivocal. According to Ref. [16], there is a single electron-like pocket covering 3% of the BZ, whereas Zhao et al. [14] report two intensity spots in the vicinity of the *X*/*Y*-point with no evidence for the electron pocket in the normal state.

In this work, we address the issue of the low energy band structure ($E \sim -300$–0 meV) of the $Ba_{1-x}K_xFe_2As_2$ superconductor and show that there are notable deviations in the FS topology as compared to the currently assumed band structure based on the available calculations. Our finding affects both the theoretical works generally aimed at reproducing the electronic structure, as well as those concentrated on a more subtle issue of superconductivity origin in the new type of superconductors. Since the FS topology also determines the loci in the reciprocal space where the superconducting gaps are to be evaluated, the correct FS topology may result in a different interpretation of current experimental data on the superconducting gaps in the novel superconductor [13–16,25]. In view of the importance of magnetic excitations in the cuprate superconductors and extended region in the phase diagram [26,27] of pnictide superconductors characterized by a spin density wave order our observations may attract attention of the scientific community to a possible common feature between the two types of unconventional superconductors.

ARPES data presented in this work were collected using synchrotron radiation ("1^3-ARPES" end station at BESSY) within the range of photon energies (20–90 eV) and various polarizations from cleaved surfaces of high quality single crystals. The overall energy and momentum resolutions were ~5 meV and

* Corresponding author. Tel.: +49 3 51 46 59 763; fax: +49 3 51 46 59 540.
E-mail address: v.zabolotnyy@ifw-dresden.de (V.B. Zabolotnyy).

0921-4534/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.physc.2009.03.043

$\sim$0.013 Å^{-1}, respectively, for the low temperature measurements. Single crystals of $Ba_{1-x}K_xFe_2As_2$ were grown using Sn as flux in a zirconia crucible sealed in a quartz ampoule filled with Ar. The mixtures of Ba, K, Fe, As and Sn in wt% ratio of ($Ba_{1-x}K_x$-Fe_2As_2):Sn = 1:85 were then heated in a box furnace up to 850 °C and kept constant for 2–4 h to soak the sample in a homogeneous melt. For growth the cooling rate of 3 °C/h was applied to decrease the temperature to 550 °C and then the grown crystals decanted from the flux.

In Fig. 1a we show experimental FS map of BKFA measured in the superconducting state at T = 10 K, which represents the photoemission intensity integrated in a small energy window $E = E_F \pm 10$ meV around the Fermi level (FL). Two concentric Γ-centered FS sheets are observed in agreement with previous studies [14,16]. Note a significant difference in the intensity distribution at different Γ points. The intensity pattern apparently repeats itself every second Γ point. This periodicity is not surprising, since such an effect is expected for a hypothetical "parent" compound with equivalent As sites. Additionally, the 3D structure of the Brillouin zone (BZ) also leads to a similar effect. In the simplest model of the photoemission the intensity distribution like the one displayed in Fig. 1a may be thought of as a cut through the 3D reciprocal space by the Ewald's sphere projected on the *kx ky* plane [28] (see panel c). At sufficiently large excitation energy, i.e. large radius of the Ewald's sphere, every second point with $k_{x,y} = 0$ would have the same k_z, while for the neighbouring points their k_z values would sum up to π/c. This, in turn, implies the periodic change of the initial state symmetry and thus photoemission intensity, when moving to a neighbouring BZ. It is important to stress that these intensity variations do not necessarily infer large k_z dispersion. On the contrary, as compared to the strong variation in the intensity distribution, the size of the Γ barrels centered at Γ_0 and $\Gamma_{\pm1}$ points turn out to be practically the same, which implies small dependence of $\varepsilon(k_x, k_y, k_z)$ on k_z. Albeit an exception [21], this is in sharp contrast with the results of most of the currently available band structure calculations [17,19,20], though inline with the anisotropy of the transport properties [29]. Further differences from the band structure calculations can be derived from the shape of the inner Γ-centered FS sheet. While in the experimental data the corners of this square-like FS sheet are directed towards the next Γ point, in the theoretical calculations the picture is rotated by 45°.

However, the major discrepancy between experiment and *ab initio* calculations is observed near the *X*/*Y*-point. According to the calculations, one expects a sizeable double-walled electron pocket. Instead, as it can be seen in Fig. 1, there is a propeller-like structure consisting of five small FS sheets near the *X*/*Y*-point: a central patch situated exactly at *X* point and four blades extended along Γ–*X* directions surrounding the central pocket. In Fig. 1b we show a similar FS map measured at T = 75 K. A detectable weakening and redistribution of intensity in the propeller-like structure can be detected above this temperature, though we find that a

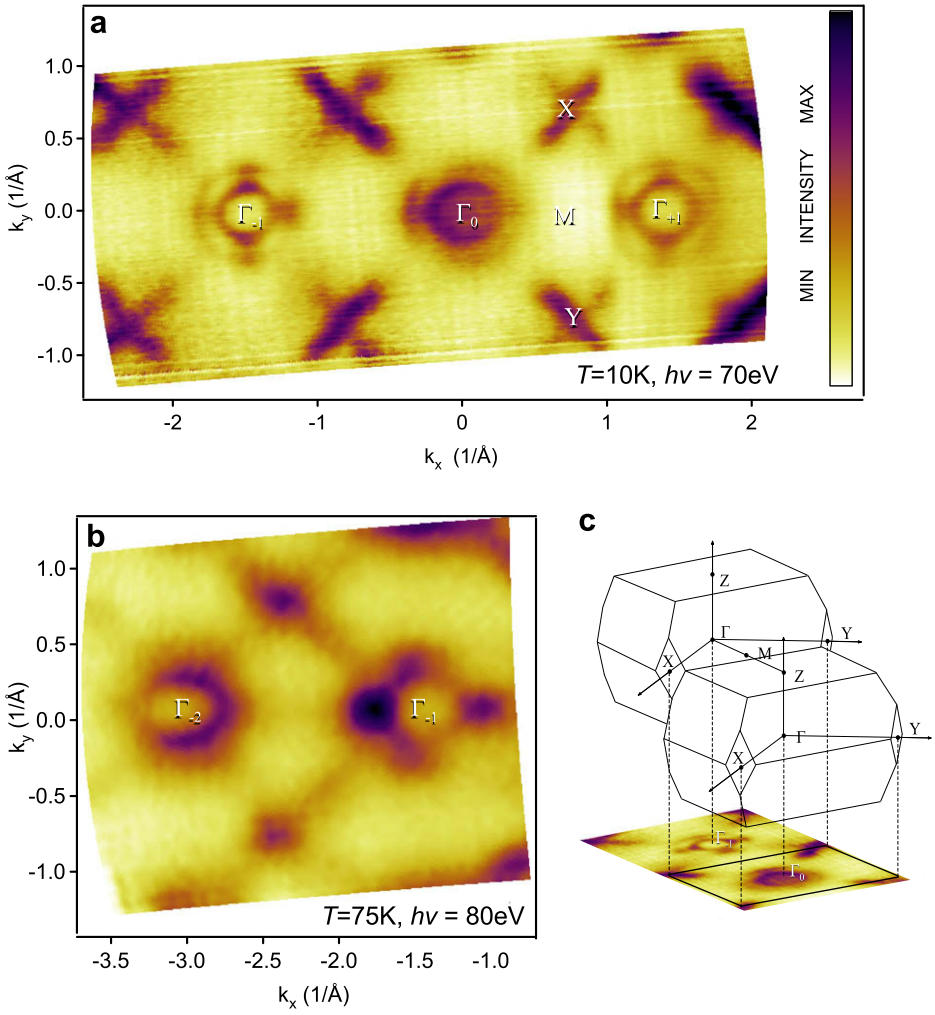

Fig. 1. (a, b) Momentum dependence of the photoemission intensity at constant energy cuts for $Ba_{1-x}K_xFe_2As_2$, at T = 10 and 75 K. (c) 3D Brillouin zone and notation of high symmetry points. When referring to ARPES data we use symbols Γ, *X*, *Y* and M as determinants for k_x and k_y values, not necessary implying the same values of k_z as in 3D case.

residual spectral weight concentrated along the 'blades' persists up to room temperature. Such temperature dependence of the intensity cannot be simply explained by the temperature broadening effects, and implies that there must be some variation in the electronic band structure. This is especially interesting in a view of the recent μSR and neutron scattering experiments [30] that show disappearance of commensurate magnetism above 70 K, implying that the new structure may result from folding caused by magnetic order [31].

To study the new structure in more detail, in Fig. 2a we present a finer FS map covering the nearest Γ and X points. To better display the dispersion of relatively broad bands, in the remaining panels (b–e) we plot the second derivative of the photoemission intensity with respect to energy as a function of quasimomentum (k_x, k_y). As can be seen the size of the blade pockets clearly increases similar to the size of the Γ barrel, signalling hole-like character of both. At the same time the feature centered exactly at the X point in the cut made at $E = 0$ meV seems to disappear, which means that its intensity must be caused by the very bottom of the electron-like pocket. This conclusion can also be supported by separate energy–momentum cuts made along the Γ–X–Γ direction as shown in Fig. 3. Depending on the light polarization one may separately enhance the photoemission either from the hole-like blades or from the electron pocket. This means that the X pocket and blades belong to different bands, since it would be unlikely for a single band to change its symmetry, i.e. its orbital character, at such a small distance in momentum space that separates the blades from the central pocket. While in the panel (b) one can find two hole bands that support the blade FS pockets situated symmetrically around X point and dispersing down below the FL, in the panel (a) the spectral weight from the X pocket is mainly concentrated in the close vicinity of the FL, which is the expected picture for a shallow electron-like band been cut by the Fermi function.

As we can now summarize, the currently available band structure calculations [17,19,20] do not reproduce the experimentally observed electronic structure exactly. Besides the issue of the k_z dispersion and form of the inner Γ-centered FS sheet, the deviations detected in the vicinity of the X/Y points are the most salient. The importance of the observed topology near the X/Y-point is that it significantly influences the density of states near the FL, which can be crucial for superconductivity [32,33]. In conclusion we want to stress that the precise knowledge of the FS allows one to understand the origin of many physical properties of a solid, like the kinetic coefficients [34], and the electronic susceptibility [35]. Details of the electronic structure determine the propensity of a

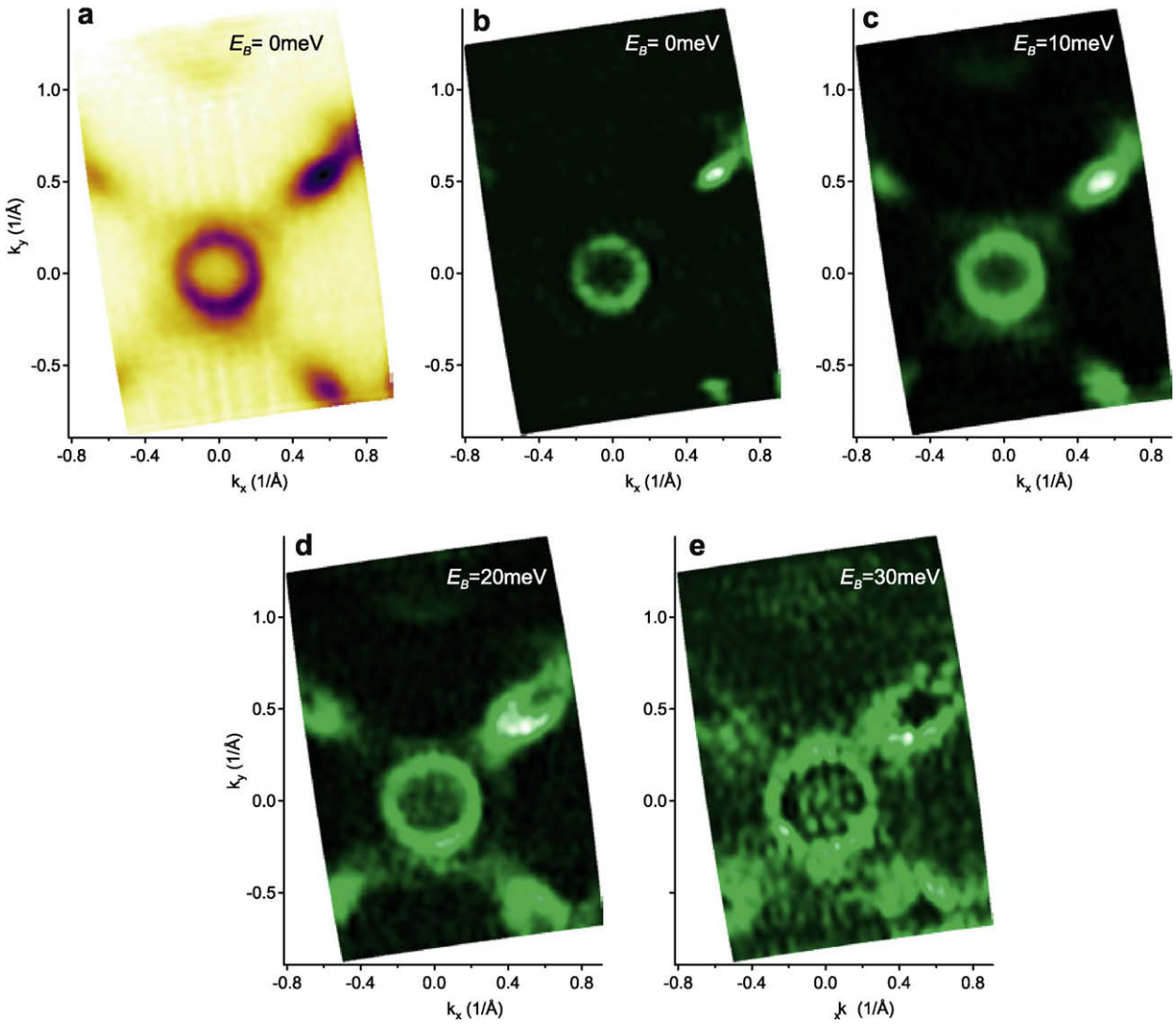

Fig. 2. (a) Fermi surface map of $Ba_{1-x}K_xFe_2As_2$, T = 15 K, $h\nu$ = 70 eV. (b–e) Second derivative of photoemission intensity with respect of energy as a function of k_x and k_y for a set of fixed energy cuts. The corresponding binding energies of the cuts are given in each panel.

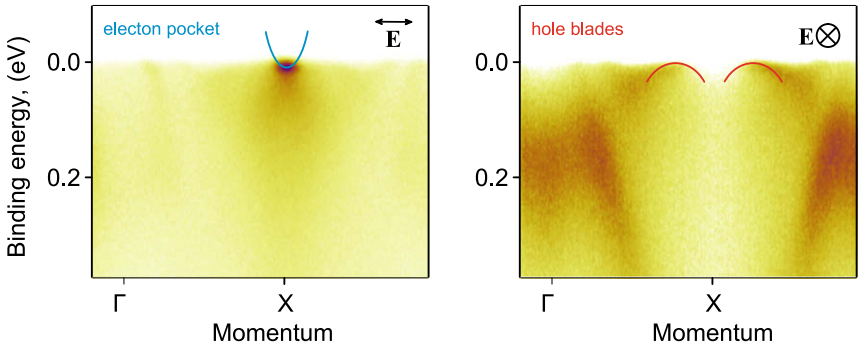

Fig. 3. Energy–momentum cut measured with different light polarization along the Γ–X–Γ direction. (a) Polarization vector of light is parallel to the analyzer slit. (b) Polarization vector perpendicular to the analyzer slit. The blue and red curves are guide to the eye corresponding to the electron pocket and blades, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

system to additional ordering [36]. In the case of superconductors, both calculations of critical temperature, as well as experimental determinations of the superconducting gap, set extremely strict requirements for the input band structure data. If doping and pressure [26,27] are so important for the superconductivity and influence first of all the shape of the FS, the precise knowledge of the low energy electronic structure will play a vital role in understanding superconductivity in the novel materials.

Acknowledgements

The project was supported, in part, by the DFG under Grant Nos. KN393/4, KN393/12 and BO 1912/2-1. We are grateful to I. Eremin, O.K. Andersen, L. Boeri, I. Mazin and M. Rümelli for fruitful discussions.

References

[1] Y. Kamihara et al., J. Am. Chem. Soc. 128 (2006) 10012.
[2] Y. Kamihara, T. Watanabe, M. Hirano, H. Hosono, J. Am. Chem. Soc. 130 (2008) 3296.
[3] H. Takahashi, Nature (London) 453 (2008) 376.
[4] H. Kito, H. Eisaki, V. Iyo, J. Phys. Soc. Japan 77 (2008) 063707.
[5] G. Wu, 2008, arXiv:/0806.1459v1.
[6] M. Rotter, M. Tegel, D. Johrendt, Phys. Rev. Lett. 101 (2008) 107006.
[7] X.H. Chen, G.W.T. Wu, R.H. Liu, D.F. Fang, Nature (London) 453 (2008) 761.
[8] G.F. Chen et al., Phys. Rev. Lett. 100 (2008) 247002.
[9] P. Richard et al., 2008, arXiv:/0808.1809v1.
[10] R. Sknepnek, G. Samolyuk, Y. bin Lee, B. Harmon, J. Schmalian, 2008, arXiv:/0807.4566v1.
[11] M.M. Parish, J. Hu, B.A. Bernevig, 2008, arXiv:/0807.4572v1.
[12] T.Y. Chen, Z. Tesanovic, R.H. Liu, X.H. Chen, C.L. Chien, Nature (London) 453 (2008) 1224.
[13] L. Wray et al., 2008, arXiv:/0808.2185v1.
[14] L. Zhao et al., Chin. Phys. Lett. 25 (2008) 4402.
[15] T. Kondo et al., Phys. Rev. Lett. 101 (2008) 147003.
[16] H. Ding et al., Europhys. Lett. 83 (2008) 47001.
[17] C. Liu et al., Phys. Rev. Lett. 101 (2008) 177005.
[18] L.X. Yang et al., 2008, arXiv:/0806.2627v2.
[19] F. Ma, Z.-Y. Lu, T. Xiang, 2008, arXiv:/0806.3526v1.
[20] D.J. Singh, 2008, arXiv:0807.2643v1.
[21] I.A. Nekrasov, Z.V. Pchelkina, M.V. Sadovskii, 2008, arXiv:0806.2630v1.
[22] D.J. Singh, M.-H. Du, Phys. Rev. Lett. 100 (2008) 237003.
[23] I.I. Mazin, D.J. Singh, M.D. Johannes, M.H. Du, Phys. Rev. Lett. 101 (2008) 057003.
[24] D.H. Lu et al., Nature (London) 455 (2008) 81.
[25] D.V. Evtushinsky et al., Phys. Rev. B 79 (2009) 054517.
[26] H. Chen et al., Europhys. Lett. 85 (2009) 17006.
[27] P.L. Alireza et al., J. Phys.: Condens. Matter 21 (2009) 012208.
[28] D. Cloetta et al., Phys. Rev. B 74 (2006) 014519.
[29] X.F. Wang et al., 2008, arXiv:/0806.2452v1.
[30] J.T. Park et al., Phys. Rev. Lett. 102 (2009) 117006.
[31] V.B. Zabolotnyy et al., Nature (London) 457 (2009) 569, doi:10.1038/nature07714.
[32] E. Cappelluti, L. Pietronero, Phys. Rev. B 53 (1996) 932.
[33] R.J. Radtke, M.R. Norman, Phys. Rev. B 50 (1994) 9554.
[34] D.V. Evtushinsky et al., Phys. Rev. Lett. 100 (2008) 236402.
[35] D.S. Inosov et al., Phys. Rev. B 75 (2007) 172505.
[36] S.V. Borisenko et al., Phys. Rev. Lett. 100 (2008) 196402.