Fermi Surfaces of the Iron-Pnictide Superconductor $BaFe_2(As_{1-x}P_x)_2$ and their Nesting Properties Revealed by Angle-Resolved Photoemission Spectroscopy

The three-dimensional shapes of the Fermi surfaces (FSs) of the iron-pnictide superconductor $BaFe_2(As_{1-x}P_x)_2$ (x=0.38), which show signatures of nodes in the superconducting gap, have been revealed by angle-resolved photoemission spectroscopy (ARPES). One of the two observed hole FSs exhibits a strong three-dimensional shape, while the other one is nearly two-dimensional. According to theories of spin fluctuation-mediated superconductivity, the observed three-dimensional shape of the FS may cause nodes in the superconducting gap.

The discovery of iron-pnictide superconductor [1] has opened up a new avenue of high-T_c research in addition to research on cuprates, bringing new challenges to the materials science community. Most of the experimental results on iron-pnictide superconductors have so far indicated that the superconducting gap opens on the entire Fermi surfaces (FSs) [2], most likely a $s\pm$-wave gap, in contrast to the d-wave superconducting gap in the high-T_c cuprate superconductors. However, recent studies on the penetration depth and thermal conductivity [3] of $BaFe_2(As_{1-x}P_x)_2$ show signatures of nodes in the superconducting gap, which may yield critical information for clarifying the pairing mechanism in iron pnictide superconductors.

According to theories of spin fluctuation-mediated superconductivity, line nodes may appear when the height of pnictogen (As or P) becomes small [4], due to changes in nesting conditions of the FSs. In fact, the importance of FS nesting for superconductivity was pointed out in early studies on iron-pnictide superconductors by angle-resolved photoemission spectroscopy (ARPES) [2]. Also, several theoretical studies predict that three-dimensional nodes in the superconducting gap may appear in a strongly warped hole Fermi surface [5, 6]. Therefore, it is crucial to reveal the three-dimensional electronic structure of $BaFe_2(As_{1-x}P_x)_2$ superconductor in order to elucidate the relationship between Fermi surface nesting, superconductivity, and gap symmetry.

We have studied the three-dimensional shapes of FSs near the optimal composition (x=0.38, T_c=28 K) by performing ARPES measurements [7]. FS mapping in the k_X-k_Y plane is shown in Fig. 1 (a). We have observed at least two hole FSs around the center of the Brillouin zone (BZ) (the Γ and Z point) and two electron FSs around the corner of the BZ (the X point). One can clearly see the small diameter of the hole FSs around the Γ point compared to those around the Z point, suggesting strong three-dimensionality of the FSs. In order to illustrate the shapes of the FSs in the k_X-k_Y plane clearly, the observed FSs are plotted in Fig. 1 (b).

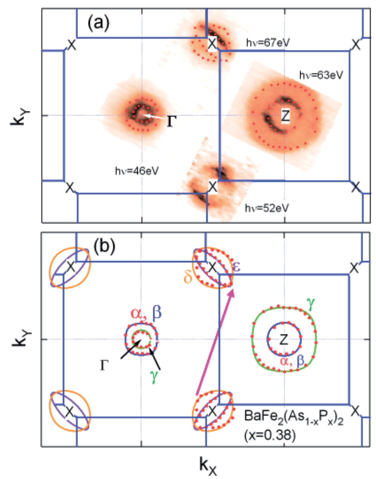

Figure 1
Fermi surfaces of $BaFe(As_{1-x}P_x)_2$ (x=0.38) observed by ARPES. (a) ARPES intensity at E_F mapped in the k_X-k_Y plane taken at several photon energies. The Brillouin zone boundary is shown by blue lines. Red dots indicate k_F positions determined by the peak positions of momentum distribution curves (MDC's). (b) Fermi surfaces determined by ARPES in the k_X-k_Y plane.

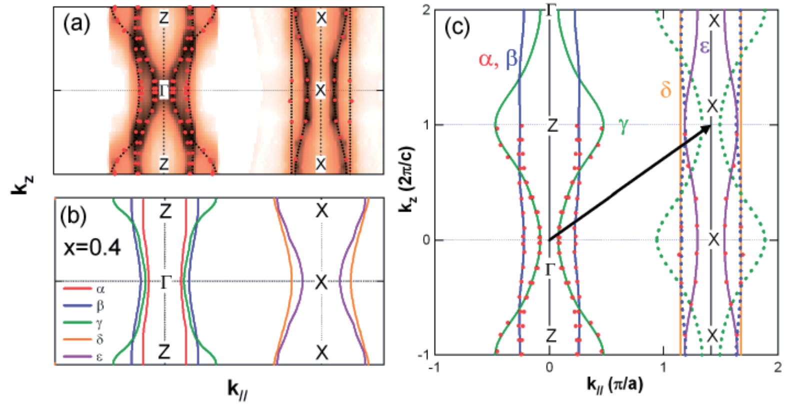

Figure 2
Hole and electron Fermi surfaces of $BaFe_2(As_{1-x}P_x)_2$ determined by ARPES in the $k_{//}$-k_z plane. (a) Result of Fermi surface mapping in the $k_{//}$-k_z plane. (b) Result of band-structure calculation for the Fermi surfaces. (c) Nesting properties of the observed FSs. Dotted lines are hole FSs shifted by the antiferromagnetic vector (black arrows).

For investigating the three-dimensional electronic structure, intensity mapping in the $k_{//}$-k_z plane was performed by changing the photon energy as shown in Fig. 2(a). Here, the direction of $k_{//}$ is parallel to the Γ-X direction. For comparison, the results of band-structure calculation for x=0.4 are shown in Fig. 2(b). We denote the hole FSs around the center of the BZ by α, β, and γ, respectively, and the outer and inner electron FSs around the corner of the BZ by δ and ε, respectively. The observed nearly two-dimensional hole FS can be assigned to the β FS with $d_{xz/yz}$ character while the three-dimensional one is assigned to γ FS with $d_{xz/yz}+d_{3z^2-r^2}$ character.

The nesting properties of the FSs based on the present results are discussed below. The shapes of the observed FSs are reproduced in Fig. 2(c) and the hole FSs shifted by the antiferromagnetic wave vector (π/a, π/a, 2π/c) are overlaid as dashed curves.

Since the β and δ FSs have different orbital character, the β-δ nesting may contribute little to the superconductivity. The γ FS shows strong warping and therefore its nesting with the electron FSs is poor. On the other hand, partial nesting between the neighboring δ electron FSs of d_{xy} orbital character persists, as indicated by the wave vector in Fig. 1(b). Since the partial nesting tends to change the sign of the gap between the nested FSs [4], nodes in the superconducting gap are likely to be realized. Alternatively, the nodes may result from partial nesting within the γ FS [5, 6]. The present results place strong constraints on the theory of the pairing mechanism and imply the importance of three-dimensional FSs in nodal superconductivity.

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