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Anisotropic Fermi surface of $BaFe_2As_2$ in the magnetostructurally ordered phase observed by angle-resolved photoemission spectroscopy

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1 Introduction

In the underdoped region of the iron pnictide superconductors, there exists an antiferromagnetic-orthorhombic (AFO) phase with a broken fourfold rotational symmetry [1]. It has been found that the major effect of doping on the AFO phase of the iron pnictides is to introduce disorder [2]. An STM study has revealed that an anomalous, anisotropic impurity state around a dopant atom is formed, which has been discussed to account for the sizable in-plane resistivity anisotropy [3]. Recently, it was surprisingly found that the sign of the resistivity anisotropy in the hole-doped systems $Ba_{1-x}K_xFe_2As_2$ and $Ca_{1-x}Na_xFe_2As_2$ reverses when $x > 0.23$ [4, 5]. Sugimoto *et al.* theoretically reproduced the sign-reversal of the in-plane resistivity anisotropy when hole was introduced, based on the interplay of impurity scattering and the anisotropic reconstructed Fermi surface (FS) in the AFO phase [6].

So far, the complete FS in the reconstructed AFO Brillouin zone (BZ) of the parent compound $BaFe_2As_2$ has been investigated using detwinned single crystals via both angle-resolved photoemission (ARPES) measurement [7] and Shubnikov-de Haas oscillation measurement [8]. However, the agreement between these experiments was limited. A schematic drawing of the 3D BZ of the body-centered tetragonal (bct) lattice for the PM state and its folded BZ for the AFO state is illustrated in Fig. 1(a). It was shown by the previous ARPES measurement that the FSs consist of two hole pockets and one electron pocket centered at the BZ center, surrounded by two bright spots along Γ-X and two bigger petal pockets along Γ-Y. On the other hand, only one hole and two electron pockets were observed by Shubnikov-de Haas oscillation measurements. Therefore, a comprehensive investigation of the FS evolution with doping has been necessary. In this study, we focus on the parent compounds $BaFe_2As_2$ and have performed an ARPES measurement of detwinned crystals.

2 Experiment

High-quality single crystals of $BaFe_2As_2$ (T_s = 142 K) were grown using the self-flux method [9]. We used a mechanical device with which a uniaxial compressive stress was applied along the tetragonal (110) direction to detwin samples in the AFO phase. ARPES experiments

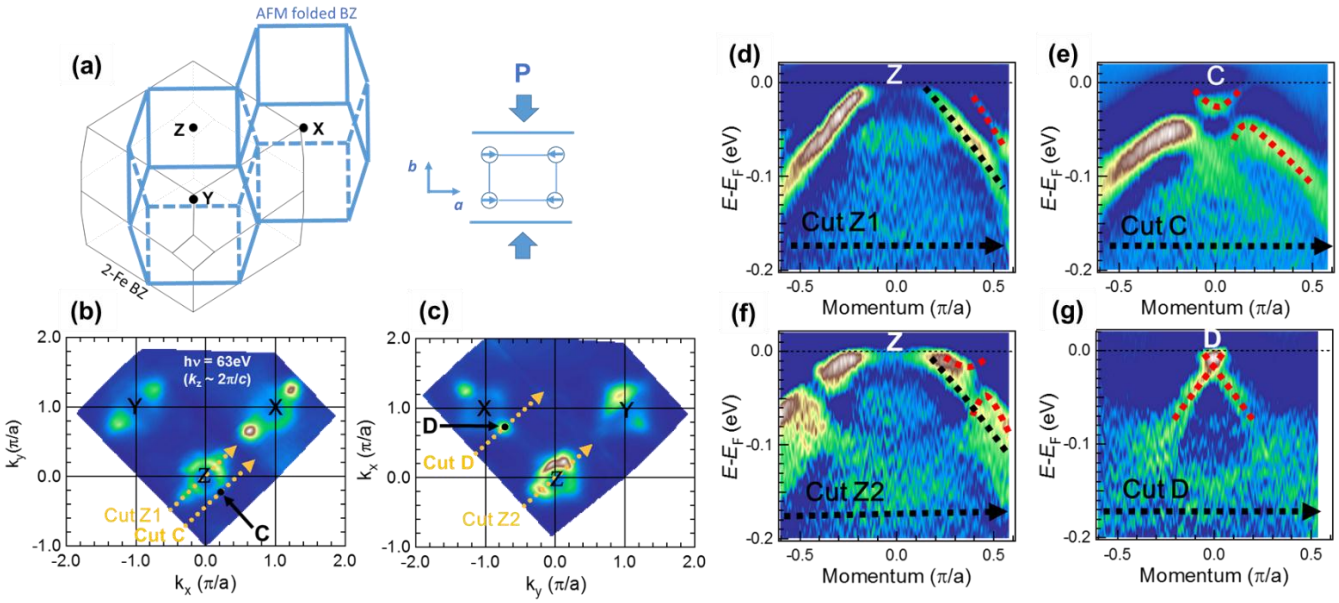

Fig. 1: Anisotropic FSs observed for detwinned $BaFe_2As_2$ single crystals in the AFO phase. (a) 3D BZ of the bct structure for the PM state (black) and that for the AFO state (blue). The right figure illustrates the crystal axes in the AFO state after detwinning by applying uniaxial pressure. (b-c) FS mapping in the k_x-k_y plane measured at 20 K. (b) was obtained by rotating the sample by 90° in the k_x-k_y plane relative to (c). (d-g) Energy second-derivatives of the energy-momentum (E-k) plots along cuts Z1, C, Z2 and D2, respectively, indicated in Fig. (b-c).

were carried out at BL 28A of Photon Factory (PF) using a SCIENTA SES2002 electron analyzer. Circularly-polarized light was used with the photon energy of 63 eV, corresponding to $k_z \sim 2\pi/c$. The total energy resolution was set to ~ 20 meV. The crystals were cleaved *in situ* at $T = 20$ K and measured in an ultra-high vacuum of ~ 1×10^{-10} Torr.

3 Results and Discussion

FS mapping in the k_x-k_y plane was performed for the detwinned crystals in the AFO state, as shown in Fig. 1(b-c), where Z-X is along the antiferromagnetic (AFM) direction and Z-Y is along the ferromagnetic direction. One can see clear anisotropy in the FS mapping intensity around the X and Y points, corresponding to the broken fourfold rotational symmetry in the AFO state. We also performed measurements with samples rotated in the k_x-k_y plane by 90°. One can see that the ARPES intensity distribution in the k_x-k_y plane is correspondingly rotated by 90°, confirming that the observed anisotropy in the FS mapping is not due to matrix-element effect but is intrinsic. We also notice the resemblance in the FS intensity map between our results and those reported by Yi *et al*. [7], indicating that the samples in our measurement were also efficiently detwinned.

Our FS mapping shows two bright spots around the X point along Z-X, one of which we denote by D. Cut D across this point shown in Fig. 1(g) demonstrates that it is a tiny electronic pocket, originating from the band crossing ~ 20 meV below E_F. The band dispersion is Dirac-cone-like. Since FSs still seem much complicated even after the problem of multi-domains have been solved by detwinning, it is difficult to determine other FS pockets. We then turn to the band dispersion, first focusing on cuts Z1 and Z2 across the Z point, as shown in Fig. 1(d, f). In both cuts, hole-like band dispersions are illustrated as a guide to the eye by black broken line. Both give the same k_F value, indicating the existence of a hole pocket with circular shape, which is consistent with the quantum oscillation measurement [8]. A clear anisotropic feature of band dispersions on the two cuts is reflected in the outer band. As for the outer band dispersion (red broken line) of cut Z2, there seems to be a gap opening, probably due to the band folding and consequent band reconstruction, which results in the formation of an electron pocket. More details of the pocket can be seen from cut C, where the band reconstruction effect is clearly demonstrated with the appearance of the gap and the formation of an electron pocket. On the other hand, cut Z1 shows only hole-like dispersion along Z-X, showing anisotropy from that of cut Z2. Because the intensity around E_F (< 20 meV) is very weak, one cannot conclude whether there is a FS pocket or not. Given the quantum oscillation results and the observed Dirac-cone like pocket surrounding X in the neighboring AFM folded BZ, it is very likely that similar Dirac-cone-like pockets are located around Z along Z-X. To summarize, our ARPES measurements show that FSs in the AFO phase consist of three types of pockets: isotropic hole pocket, Dirac-cone-like tiny electron pockets along Z-X and another electron pocket along Z-Y originating from the AFM ordering, which is consistent with that reached by the quantum oscillation measurement [8].

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