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Three-dimensional electronic structure of $FeTe_{0.6}Se_{0.4}$

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1 Introduction

The electronic structures of iron-based superconductors have been intensively studied since their discovery, and from the early stage, their three dimensionality has been recognized as one of the most important difference from the highly two-dimensional high-T_c cuprates [1]. As for the 11-type compounds such as Fe(Te,Se), from the laser-based angle-resolved photoemission spectroscopy (laser AREPS) , it has been reported that only one hole band crosses the Fermi level (E_F) around the Γ point of the Brillouin zone (BZ), while an electron band was found just above E_F at the Γ point [2]. This is a significant difference from the predictions from the band-structure calculations based on the density functional theory (DFT) that three hole Fermi surfaces (FSs) exist around the Γ point. Hence, it is important to further investigate the difference between the actual three-dimensional electronic structure and the DFT results.

2 Experiment

ARPES measurements were performed at BL-28A of Photon Factroy (PF) with the photon energies from 35 eV to 90 eV. High-quality single crystals of $FeTe_{0.6}Se_{0.4}$ were grown by a melt-growth technique. The superconducting transition temperature (T_c) was confirmed to be ~ 14 K. More details were described in the literature[3]. Lattice constants were taken from a literature for the same composition [4]. Clean surfaces were obtained by cleaving the samples *in situ*. The measurements were performed at the temperature of 25 K (> T_c) in an ultra-high vacuum of ~ 2×10^{-8} Pa.

3 Results and Discussion

Figure 1 shows the result of FS mapping in the $k_{//}$-k_z plane for $FeTe_{0.6}Se_{0.4}$. The momentum perpendicular to the surface k_z was deduced assuming a free-electron final state. From the periodic modulation of the intensity at E_F, the value of the inner potential was determined as 12 eV, which is similar to those of other iron-based superconductors [5]. From this value of the inner potential, 44 eV, 59 eV and 76 eV correspond to the Z, Γ, and Z points of the BZ, respectively. By measuring band dispersions with these photon energies, we concluded that any significant three-dimensionality cannot be found in $FeTe_{0.6}Se_{0.4}$. Combined with the result of the laser ARPES that only one hole band crosses the E_F around the Γ point,

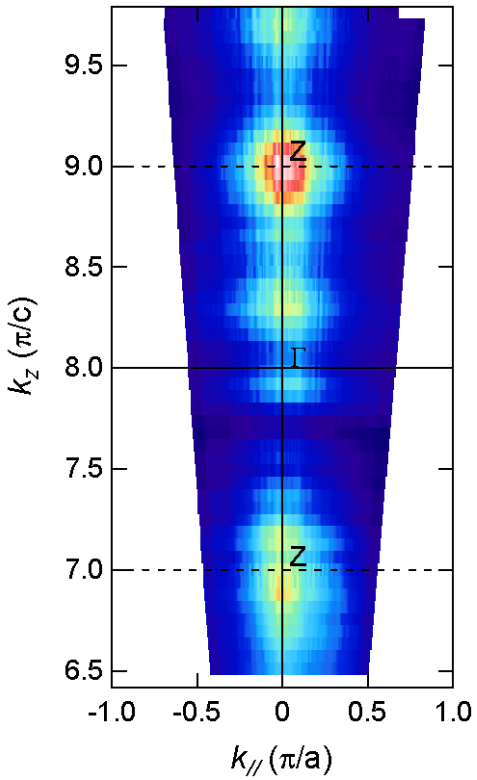

Fig. 1: Fermi-surface mapping of $Fe_{Te0.6}Se_{0.4}$ in the $k_{//}$-k_z plane.

it is suggested that only one hole FS exists in the entire BZ for $FeTe_{0.6}Se_{0.4}$.

References

[1] W. Malaeb, *et al* . *J. Phys. Soc. Jpn.* **78,** 123706 (2009).
[2] K. Okazaki *et al*., *Sci. Rep.* **4**, 4109 (2014).
[3] K. Okazaki *et al. Phys. Rev. Lett.* **109**, 237001 (2012).
[4] S. Li *et al.*, *Phys. Rev. B* **79**, 054503 (2009).
[5] T. Yoshida *et al.*, *Frontiers in Physics* **2**, 17 (2014).

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