BL-2A/Commissioning

Band structure of the weakly ferromagnetic superconductor $Sr_2VFeAsO_{3-\delta}$

Masafumi Horio[1,*], Takao Katagiri[2], Hiromitsu Namiki[2], Kozo Okazaki[1], Hakuto Suzuki[1], Jian Xu[1], Keisuke Koshiishi[1], Masaki Kobayashi[3], Makoto Minohara[3], Enju Sakai[3], Koji Horiba[3], Hiroshi Kumigashira[3], Takao Sasagawa[2] and Atsushi Fujimori[1]
[1]Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan
[2]Materials and Structures Laboratory, Tokyo Institute of Technology, Yokohama, Kanagawa 226-8503, Japan
[3] Photon Factory, KEK, Tsukuba, Ibaraki 305-0801, Japan

1 Introduction

The iron-based superconductor $Sr_2VFeAsO_{3-\delta}$ shows a relatively high superconducting transition temperature (T_c) of 37 K for $\delta = 0$ [1]. While the Fe 3*d* electrons in the FeAs layer are certainly responsible for the superconductivity, a Mott-insulator-like behavior has been proposed for the V 3*d* electrons in the Sr_2VO_3 layer [2]. When oxygen deficiencies of $\delta = 0.5$ are introduced, T_c decreases to 20 K and a weak ferromagnetism appears with a Curie temperature of $T_C \sim 240$ K and a magnetic moment of $\sim$ 0.1 μ_B/V [3]. Although the weak ferromagnetism has been attributed to the canted magnetic moment of the V atom, the origin of the ferromagnetism is still unknown. Also, the oxygen-deficiency-induced changes in the electronic structure have not been studied so far.

In this work, we have performed angle-resolved photoemission spectroscopy (ARPES) measurements on single crystals of ferromagnetic $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0.5$) by use of photons with different polarizations to elucidate the band structure including its orbital character.

2 Experiment

Single crystals of $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0.5$) were grown by the self-flux method. The superconducting transition temperature T_c, which was determined by magnetic susceptibility measurements, was 14 K, and the Curie temperature T_C was 240 K.

ARPES measurements were carried out at BL-2A of Photon Factory using linearly polarized light parallel (*p* polarization) and perpendicular (*s* polarization) to the mirror plane with $h\nu = 72$ eV. A SCIENTA SES-2002 analyzer was used with the total energy resolution of 35 meV. Single crystals were cleaved *in-situ* in the vacuum of $\sim 1 \times 10^{-10}$ Torr at $T = 22$ K. Samples were oriented as described in Fig. 1. Here, *X* and *Y* are parallel to the crystal axis, and *x* and *y* are parallel to the nearest-neighbor Fe-Fe direction.

3 Results and Discussion

Fig. 2 shows Fermi surfaces and intensity plot in energy-momentum space along the Γ-M line. Clear

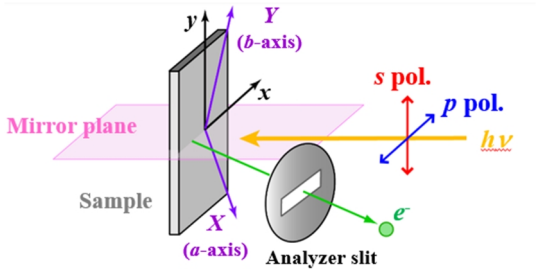

Fig. 1 Experimental setup for the ARPES measurements. *X* and *Y* are parallel to the crystallographic a and b axes, and *x* and *y* are parallel to the nearest-neighbor Fe-Fe directions.

differences in the intensity distribution are observed between the intensity plots taken with *s* and *p* polarization reflecting the selection rule: photons with *s* polarization excite electrons from d_{yz} and d_{xy} orbitals, while excitation occurs from d_{xz}, d_{x2-y2}, and d_{3z2-r2} orbitals with *p* polarization. By extracting peak positions in energy distribution curves (EDCs) and momentum distribution curves (MDCs), band structure has been deduced as shown in Fig. 3(a).

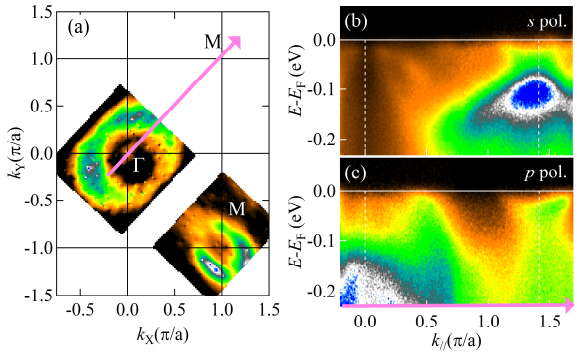

Fig. 2 ARPES spectra of $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0.5$). (a) Fermi surfaces. (b), (c) Intensity plots in energy-momentum space taken with *s* and *p* polarizations, respectively along the Γ-M line shown in (a).

Experimentally derived band dispersions were further compared to those calculated within density functional theory (DFT) using a Wien2k program as shown in Figs. 3(b) and (c). Although in the previous study [2] it has been claimed that the near-E_F band structure can be explained only by Fe 3*d* orbitals in the paramagnetic state in the stoichiometric sample $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0$), it is not the case for the present $\delta = 0.5$ sample. Some of the bands can be attributed to Fe 3*d* orbitals, but the other bands around the zone center still remain unassigned. One explanation for the observed complicated band structure is the antiferromagnetic ordering of Fe. According to an NMR study it has indeed been claimed that Fe is in the antiferromagnetic state below 165 K [4]. However, this is less likely in the present sample because the band dispersion around the M point, which could be folded in a complicated way with antiferromagnetic order, can be described by the calculation for the paramagnetic state. Another possibility is that the V 3*d* bands were observed around the zone center. DFT calculation actually supports the existence of V $d_{YZ/XZ}$ and d_{XY} bands near the zone center as shown in Fig. 3(c), and the experimentally obtained bands in the region $|k_{//}| < 0.5$ (π/a) are reasonably reproduced by considering the V $d_{YZ/XZ}$ orbitals. Two bands which still cannot be assigned (α and β in Fig. 3(d)) would be d_{XY} and $d_{YZ/XZ}$ bands, respectively, which were scattered by magnetic order found in the V atom [5,6] or oxygen vacancies if they are periodically ordered.

In conclusion, we have performed ARPES measurements on the weakly ferromagnetic superconductor $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0.5$) using different photon polarizations and observed band dispersions orbital-selectively. Obtained band structures were reproduced by considering not only Fe 3*d* but also V 3*d* bands.

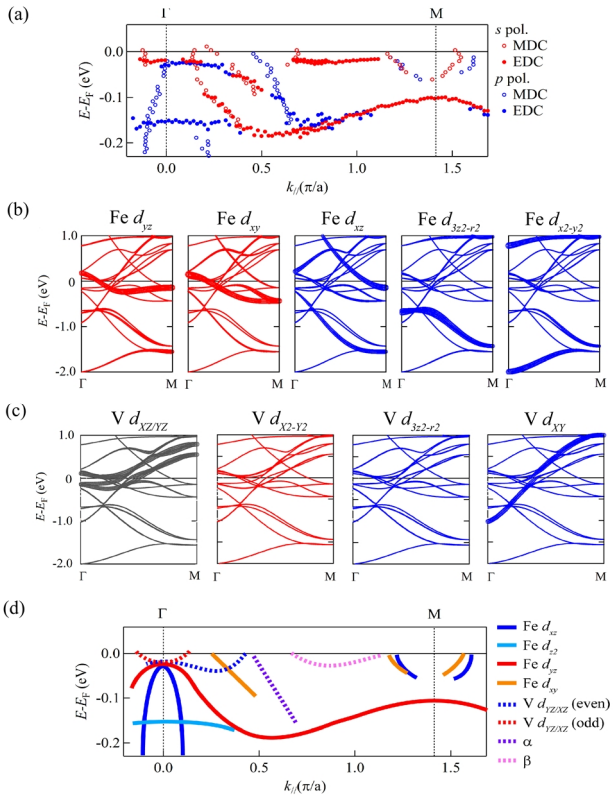

Fig. 3 Comparison between experimental and calculated band structure. (a) Peak positions in MDCs and EDCs extracted from Fig. 1(b) and (c). (b), (c) Band dispersion near E_F calculated using a Wien2k program. The thickness of the band corresponds to the weight of the indicated Fe or V 3*d* orbital character. Red and blue thick bands can be observed with *s* and *p* polarization, respectively. (d) Schematically drawn experimental band structure with orbital character assignment.

References

[1] X. Zhu *et al.*, Phys. Rev. B. **79**, 220512(R) (2009).
[2] T. Qian *et al.*, Phys. Rev. B. **83**, 140513 (2011).
[3] T. Katagiri *et al.*, 25pEC-2, JPS autumn meeting (2013).
[4] K. Ueshima *et al.*, Phys. Rev. B. **89**, 184506 (2014).
[5] M. Tegel *et al.*, Phys. Rev. B 82, 140507(R) (2010).
[6] F. Hummel *et al.*, Phys. Rev. B 88, 144517(R) (2013).

* horio@wyvern.phys.s.u-tokyo.ac.jp