BL-28A/2012S2-001,2013G218, BL-2A, BL-16A/2013S2-004

ARPES and core-level spectroscopies of the coexistence of ferromagnetism and superconductivity in $Sr_2VFeAsO_{3-\delta}$

Masafumi Horio[1,*], Kozo Okazaki[1], Takao Katagiri[2], Hakuto Suzuki[1], Jian Xu[1], Keisuke Ishigami[1], Yukio Takahashi[1], Goro Shibata[1], Shoya Sakamoto[1], Kanta Ono[3], Hiroshi Kumigashira[3], Koji Horiba[3], Masaki Kobayashi[3], Enju Sakai[3], Tsuneharu Koide[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 responsible for the superconductivity, 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 $\sim 0.1 \mu_B$/V [3]. Although this weak ferromagnetism has been associated with a 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) and core-level spectroscopy measurements on single crystals of $Sr_2VFeAsO_{3-\delta}$ with different amount of oxygen deficiencies ($\delta = 0$ and 0.5).

2 Experimental

Single crystals of $Sr_2VFeAsO_{3-\delta}$ ($\delta = 0$ and 0.5) were grown by the self-flux method. The superconducting transition temperature T_c, which was determined by magnetic susceptibility measurements, was 27 K and 14 K, and Curie temperature T_C was 0 K and 240 K for the $\delta = 0$ and 0.5 samples, respectively.

ARPES measurements were carried out at BL-28A of Photon Factory using circularly and linearly polarized light with $h\nu$ = 58 eV and 80 eV. X-ray photoemission spectroscopy (XPS) measurements were made at BL-2A of Photon Factory using linearly polarized light with $h\nu$ = 1100 eV. A SCIENTA SES-2002 analyzer was used with the total energy resolution of 30-40 meV and 300 meV at BL-28A and BL-2A, respectively. X-ray absorption spectroscopy (XAS) were performed at BL-2A and BL-16A of Photon Factory in the total electron yield (TEY) mode using linearly and circularly polarized light, respectively. Single crystals were cleaved *in-situ* in the vacuum of $\sim 1 \times 10^{-10}$ Torr at $T = 40$ K.

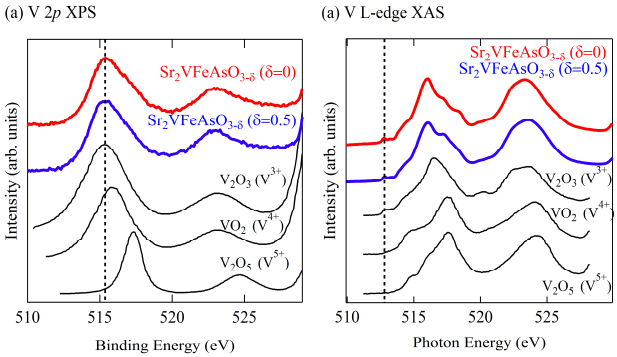

Fig. 1: Core-level spectra of $Sr_2VFeAsO_{3-\delta}$. (a) V 2*p* XPS. (b) V *L*-edge XAS.

3 Results and Discussion

In Fig. 1, V 2*p* XPS and V *L*-edge XAS spectra are plotted with reference spectra of other vanadium oxides. The peak position of the V 2*p* core level in the XPS spectra was close to that of V_2O_3 for both of $\delta = 0$ and $\delta = 0.5$ samples. In addition, XAS spectra of both samples showed a peak at $\sim$ 512.5 eV similarly to V_2O_3, and hence the valence of V in $Sr_2VFeAsO_{3-\delta}$ was close to 3+, regardless of the amount of the oxygen deficiencies.

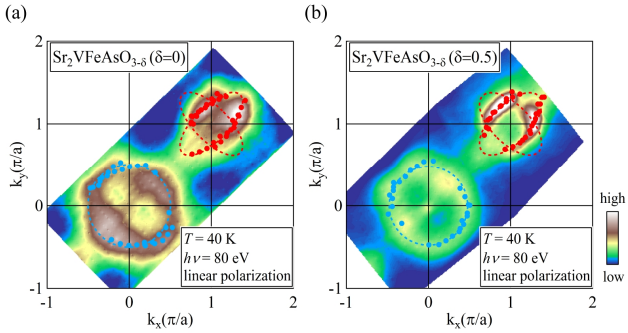

Fig. 2: Fermi surface mappings for the $\delta = 0$(a) and the $\delta = 0.5$ (b) samples, respectively. The positions of k_F are indicated by closed dots.

Fermi surface (FS) mapping is shown in Fig. 2. In both samples, large hole and electron FSs were observed at the Brillouin zone (BZ) center and corner, respectively. The FS area was 19.8 % of the 1st BZ for the hole FS and 15.6 %

for the electron FS in the δ = 0 sample, which amounts to 4.2 % hole excess. On the other hand in the δ = 0.5 sample, the area of the hole and electron FSs are 17.9 % and 16.9 %, respectively, which means 1.0 % holes excess, which is not so much different from that of the δ = 0 sample.

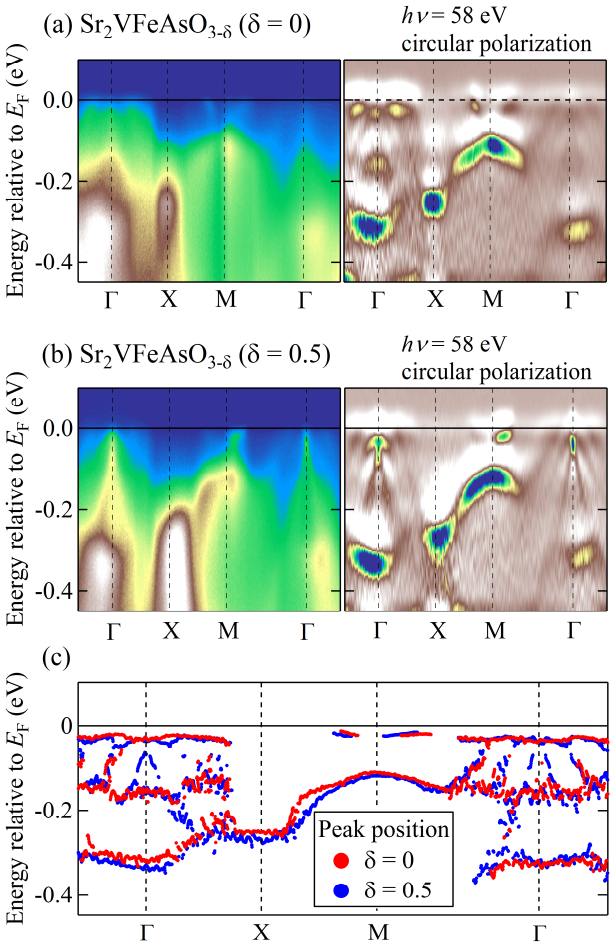

Fig. 3: Band dispersions along high-symmetry lines in the BZ. (a) ARPES spectra (left) and its second energy derivative for the δ = 0 sample (right). (b) The same as (a) for the δ = 0.5 sample. (c) Plot of the negative peak positions of the second derivative spectra extracted from (a) and (b).

Not only the size of the FS but also the overall band position did not change significantly with oxygen deficiencies as one can see from Fig. 3, where the second energy derivatives of the ARPES spectra and their negative peak positions are plotted. Instead, clear difference was observed in the spectral intensity of the band below ~ 0.15 eV at the BZ center.

In order to examine the detailed band structure near E_F, energy-momentum plot and its second energy derivative for both samples are displayed in Figs. 4(a) and (b). Although two bands with very steep dispersions crossing at ~ -0.05 eV were clearly observed around $k_{//} \sim 0$ in the δ = 0.5 sample, the corresponding bands in the δ = 0 sample were far less intense than that in the δ = 0.5 one.

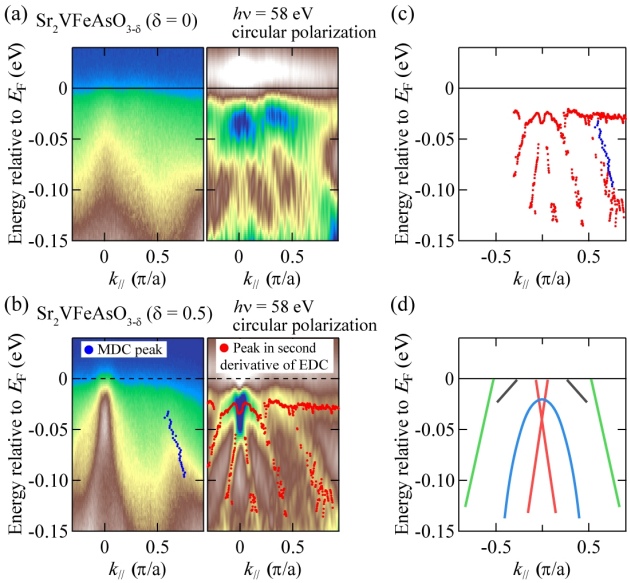

Fig. 4: Band structure near E_F around the BZ center. (a) ARPES spectra of the δ = 0 sample (left) and its second derivative in energy direction. (b) The same as (a) for the δ = 0.5 sample. Peak positions of MDC and second derivative of EDC are also plotted in left and right panels, respectively. (c) The peak positions extracted from (b). (d) Schematic band structure of the δ = 0.5 sample near the BZ center described in accordance with the peak position shown in (c).

Considering the fact that these pronounced bands were not observed also in a δ = 0 sample measured in a previous ARPES study [2], they should be a new feature induced by the oxygen deficiency. In Figs. 4(c) and (d), peak positions of the momentum distribution curves (MDCs) and the second derivative of energy distribution curve (EDC) for the δ = 0.5 sample, and thus determined schematic band structure are shown, respectively. At least five bands are observed near the BZ center, which cannot be accounted for by a previous local density approximation (LDA) + U calculation in which it is assumed that only Fe 3d bands lay near E_F while V 3d electrons were in a Mott insulating state [2]. We propose that V 3d electrons form energy bands near E_F at least in the δ = 0.5 sample.

In conclusion, we have performed core-level spectroscopy and ARPES measurements on single crystals of $Sr_2VFeAsO_{3-\delta}$ (δ = 0 and 0.5). Although oxygen deficiencies were supposed to dope electrons, clear difference was not seen either in XPS spectra or in the FS area between the δ = 0 and 0.5 samples. The spectral intensity of the band around the BZ center near E_F was strongly enhanced by the oxygen deficiency. Because the observed band structure of the δ = 0.5 sample could not be reproduced by the LDA + U calculation which assumed that V is in a Mott insulating state, V 3d electrons are found to form energy bands around E_F.

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).

Research Achievements (optional)
1. IMSS Science Festa 2013, Poster presentation prize (2013).

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