ARPES and core-level spectroscopies of the coexistence of ferromagnetism and superconductivity in Sr$_2$VFeAsO$_{3-\delta}$

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1 Introduction

The iron-based superconductor Sr$_2$VFeAsO$_{3-\delta}$ 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$_2$VO$_3$ 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 $T_C \sim 240$ 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$_2$VFeAsO$_{3-\delta}$ with different amount of oxygen deficiencies ($\delta = 0$ and 0.5).

2 Experimental

Single crystals of Sr$_2$VFeAsO$_{3-\delta}$ ($\delta = 0$ 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.

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$_2$O$_3$ 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$_2$O$_3$, and hence the valence of V in Sr$_2$VFeAsO$_{3-\delta}$ was close to 3+, regardless of the amount of the oxygen deficiencies.

Fig. 1: Core-level spectra of Sr$_2$VFeAsO$_{3-\delta}$. (a) V 2$p$ XPS. (b) V L-edge XAS.

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

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 \( k_\perp \sim 0 \) in the \( \delta = 0.5 \) sample, the corresponding bands in the \( \delta = 0 \) sample were far less intense than that in the \( \delta = 0.5 \) one.

Considering the fact that these pronounced bands were not observed also in a \( \delta = 0 \) 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 \( \delta = 0.5 \) 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 \( \delta = 0.5 \) sample.

In conclusion, we have performed core-level spectroscopy and ARPES measurements on single crystals of \( \text{Sr}_2\text{VFeAsO}_5 \) (\( \delta = 0 \) 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 \( \delta = 0 \) 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 \( \delta = 0.5 \) 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

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

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