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Electronic structure of $Ba(Fe_{0.96}Zn_{0.04})_2As_2$ with antiferromagnetic ordering

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1 Introduction

One of the parent compounds in iron-based superconductors $BaFe_2As_2$ (Ba122) is an antiferromagnetic metal below the Néel temperature (T_N), and becomes superconducting (SC) by the substitution of transition-metal atoms such as Co, Ni, and Cu for Fe [1, 2, 3, 4]. This is a remarkable phenomenon given the fact that the substitution of transition-metal atoms in the CuO_2 plane of the cuprate superconductors quickly kill the superconductivity [5]. According to the rigid-band model, the substitution leads to electron doping and the doped electron number in $Ba(Fe_{1-x}Co_x)_2As_2$ (Co-Ba122), $Ba(Fe_{1-x}Ni_x)_2As_2$ (Ni-Ba122), and $Ba(Fe_{1-x}Cu_x)_2As_2$ (Cu-Ba122) is expected to be x, $2x$, and $3x$, respectively. Experimental studies have shown that the electrons are indeed doped by substitution of Co, Ni, and Cu for Fe, and the electronic structure may show the rigid-band model [2, 4]. However, according to a recent calculation on supercells [7, 8], the extra electronic charges are largely distributed on the substituted Co, Ni, Cu or Zn atoms, apparently contradicting with the rigid-band model.

Recently, our angle-resolved photoemission spectroscopy (ARPES) study has revealed that the electronic structure of the transition-metal doped Ba122 is deviated from the rigid-band model in going from Co-, Ni-, to Cu-Ba122 due to the increasing strength of the impurity potential, and hence part of the doped electrons may not participate in the formation for the Fermi surfaces [6]. This also indicates that the impurity potential is one of the key factors to determine the T_c of the electron-doped iron-based superconductors. However, an interesting question still remains: Zn doped $Ba(Fe_{1-x}Co_x)_2As_2$ and $LaFeAsO_{1-x}F_x$ still show a relatively high T_c [9, 10], although Zn is one of the strong scatteres and this compound is expected to be heavily electron doped. It is an intriguing issue to elucidate why the Zn atom does not destroy the superconductivity.

We have performed an ARPES measurement to investigate the electronic structure on $Ba(Fe_{0.96}Zn_{0.04})_2As_2$ (Zn-Ba122). We find that hole and electron Fermi surfaces (FSs) show a band folding due to the antiferromagnetic ordering below T_N with little indication of carrier doping, and the electronic structure of Zn-Ba122 does not agree with the rigid-band model.

2 Experiment

High-quality single crystals of Zn-Ba122 with $x = 0.04$ were grown by the self-flux method. ARPES measurements were carried out at beamline 28A of Photon Factory (PF) using linearly-polarized light. The crystals were cleaved *in situ* at $T = 20$ K in an ultra-high vacuum of 5×10^{-11} Torr.

3 Results and Discussion

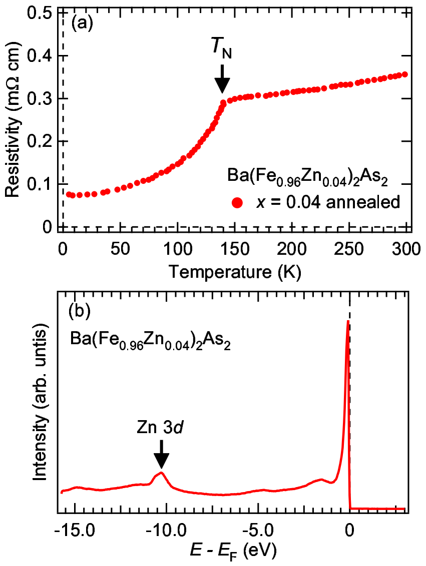

Fig. 1: (a): *ab*-plane resistivity as a function of temperature for annealed Zn-Ba122. (b): Valence-band spectrum taken at $h\nu = 60$ eV and $T = 20$ K.

Figures 1(a) and 1(b) show respectively the resistivity and the valence-band spectrum observed by angle-integrated photoemission spectroscopy of Zn-Ba122 with $x = 0.04$. One can see that the resistivity shows a kink around $T\sim 140$ K, which corresponds to the magnetic phase transition like the parent compound

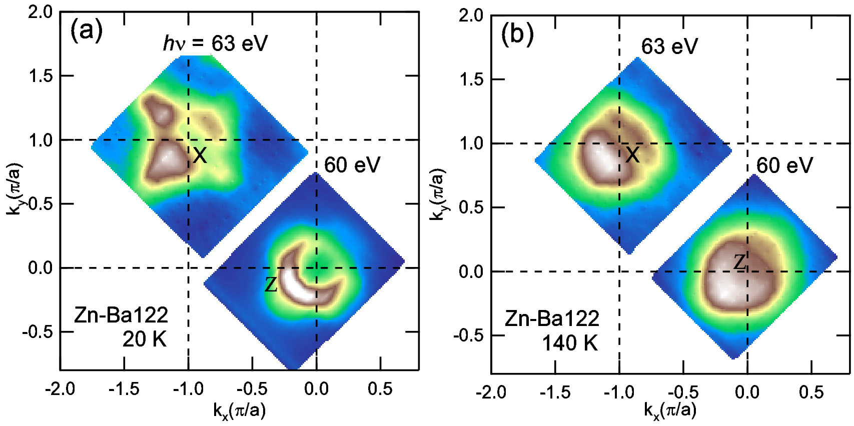

Fig. 2: ARPES intensity map in the two-dimensional k_x-k_y plane for Ba(Fe$_{0.96}$Zn$_{0.04}$)$_2$As$_2$ (Zn-Ba122) taken at T = 20 and 140 K.

BaFe$_2$As$_2$. The valence-band spectrum is shown in Fig. 1(b), and the Zn 3*d* band appears around 10 eV below Fermi level as shown by a black arrow. The binding energy of the Zn 3*d* band is consistent with the band-structure calculation [7]. From analogy to the previous ARPES study [6], one can expect that Zn-Ba122 does not follow the rigid-band model due to the strong impurity potential.

We show an ARPES intensity plot of Zn-Ba122 taken at T = 20 and 140 K in Figs. 2(a) and 2(b), respectively. One finds that the shapes of the hole and electron FSs are similar to those of parent compound, namely, small pockets are observed as expected for zone folding after the spin density wave formation. One may expect that the doped Zn atoms donate four times as large number of electrons as that in the case of Co atom. However, the hole FSs are clearly observed. Therefore, in the case of Zn doping, the doped electrons do not supply carriers into the Fe 3*d* band. Hence, we can conclude that the rigid-band model fails in Zn-Ba122.

In conclusion, we have performed an ARPES study to investigate the electronic structure of the electron-doped Ba(Fe$_{0.96}$Zn$_{0.04}$)$_2$As$_2$. We have found that the shape and the area of the hole and electron FSs does not change apparently from the parent compound BaFe$_2$As$_2$. This is due to the strong impurity potential of the Zn atom which localizes all the doped electrons at the Zn site.

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