Electronic structure of Zn-substituted BaFe₂As₂ revealed by angle-resolved photoemission spectroscopy

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1 Introduction

The role of substituted transition-metal atoms in the electronic structure has been one of the most important but difficult issues in the iron-based superconductors (Fe-SCs). Based on supercell calculations within the density functional theory (DFT), Wadati *et al.* have studied the spatial distribution of extra electrons in Co-, Ni-, Cu-, and Zn-substituted BaFe₂As₂ and found that the extra electrons are located at the Co, Ni, Cu, and Zn sites [1]. Our recent angle-resolved photoemission spectroscopy (ARPES) measurement has revealed that deviation from the rigid-band model gradually develops in going from Co-, Ni-, to Cu-substituted BaFe₂As₂ [2]. For Zn substitution, according to the rigid-band model, the doped electron number is expected to be four times as large as that of Co doping, and at the same time the impurity potential is expected to be stronger than Co, Ni, and Cu. Here, we report the electronic structure of Zn-doped BaFe₂As₂ revealed by ARPES [3].

2 Experiment

High-quality single crystals of Ba(Fe₁₋ₓZnₓ)₂As₂ with x = 0.08 and 0.25 were grown by the self-flux method. The Zn concentration was determined by energy dispersive X-ray (EDX) analysis. ARPES measurements were carried out at beamline 28A of Photon Factory using linearly polarized light ranging from hv = 34–80 eV. A Scienta SES-2002 analyzer was used with the total energy resolution of 15–20 meV. The crystals were cleaved *in situ* at T = 20 K in an ultrahigh vacuum of ~5 × 10⁻¹¹ Torr.

3 Results and Discussion

In order to estimate the FS volumes quantitatively, Fermi surface (FS) mapping in the k_z-$k_\parallel$ plane was performed by changing the photon energy as shown in Fig. 1. Here, the intensity asymmetry observed with respect to the $k_\parallel$ = 0 line is due to photoemission matrix-element effects. Figures 1(a) and 1(c) show the hole FS mapping on the k_z-$k_\parallel$ plane at T = 20 K for the x = 0.08 and 0.25 samples, respectively, and Figs. 1(b) and 1(d) are their second derivatives. With changing photon energy,
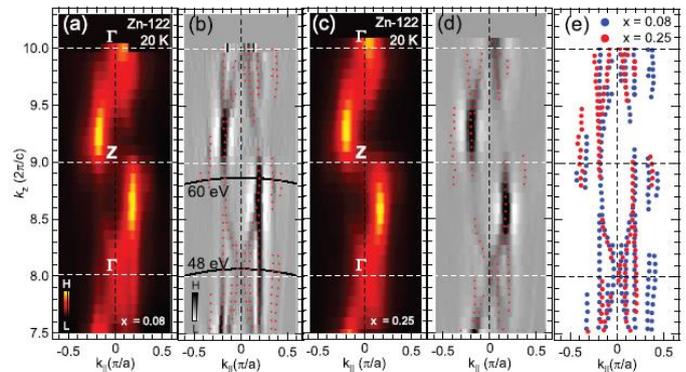

Fig. 1: Fermi-surface mapping of Zn-substituted BaFe₂As₂ in the $k_\parallel$-k_z plane below T_N ~ 135 K. (a), (c) Hole FSs around the center of the Brillouin zone. (b), (d) Second-derivatives of the intensity maps in (a) and (c), respectively. Red dots denote positions of the Fermi momentum (k_F). k_F's deduced from panels (b) and (d) are shown in panel (e).

the hole FSs show strong three dimensionality, and are folded due to antiferromagnetic order [3], similar to the previous ARPES and de Haas–van Alphen studies of BaFe₂As₂ [4,5]. This indicates that the electronic structure of BaFe₂As₂ near the Fermi level (E_F) is not affected by the Zn substitution because the strong impurity potential of Zn binds all the extra 3*d* electrons around -10 eV below the E_F.

References
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