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Fermi surfaces of the iron-based superconductor $Ba(Fe_{1-x}Cu_x)_2As_2$ observed by angle-resolved photoemission spectroscopy

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Introduction

The electron-doped iron-based superconductor $Ba(Fe_{1-x}TM_x)_2As_2$ (TM = Ni, Cu) shows superconductivity and the maximum superconducting transition temperature reaches ~ 18 K at x ~ 0.05 (*TM* = Ni) and ~ 2 K at x ~ 0.044 (TM = Cu) [1, 2]. In $Ba(Fe_{1-x}Ni_x)_2As_2$ [$Ba(Fe_{1-x}Cu_x)_2As_2$], it is expected that the electron carrier concentration is twice (three times) as large as that of $Ba(Fe_{1-x}Co_x)_2As_2$. In previous angle-resolved photoemission spectroscopy (ARPES) studies of $Ba(Fe_{1-x}Co_x)_2As_2$, the superconducting gaps [3] and the three-dimensional hole and electron Fermi surfaces (FSs) [4, 5] have been observed. Also, the shift of chemical potential and the number of hole and electron carriers have been estimated from the ARPES data, and interpreted by the rigid-band picture [5]. On the other hand, according to theoretical calculation, the doped *d* electrons due to the caused by impurity atoms such as Co, Ni and Cu are almost located within the muffin-tin sphere of the substituted site [6]. Therefore, the calculation is inconsistent with the rigid-band picture observed in the previous ARPES studies [5]. In this work, we have studied the electronic structure of $Ba(Fe_{1-x}Cu_x)_2As_2$ with Cu concentration x = 0.04, 0.06 and 0.08. Particularly, we focused on the photon-energy dependence of ARPES spectra.

Experimental Condition

High-quality single crystals of non-superconducting $Ba(Fe_{1-x}Cu_x)_2As_2$ with x = 0.04, 0.06, and 0.08 were grown by self-flux method. ARPES measurements were carried out at Beamline 28A of Photon Factory (PF) using circularly-polarized light from h = 34 to 88 eV. A Scienta SES-2002 analyzer was used with the total energy resolution of ~15 meV and the momentum resolution of ~ 0.02π/a. In-plane (k_x, k_y) and out-of-plane electron momenta (k_z) are expressed in units of π/a and 2π/c, respectively, where a and c are the in-plane and out-of-plane lattice constants. The crystals were cleaved *in situ* at T ~ 10 K under an ultra-high vacuum of ~ 6×10^{-11} Torr.

Results and Discussion

Figure 1 shows the result of the mapping of the electron FSs for the optimally doped to overdoped Cu-Ba122 taken at T = 9 K. We find that the hole FS along the Γ-Z direction disappears as a result of electron doping for all compositions. We have also found that the volume of the electron FS does not show a large difference between the different Cu concentrations. This result implies that the doped electron carriers by the Cu substitution are trapped around the impurity sites, and does not follow a simple rigid-band shift.

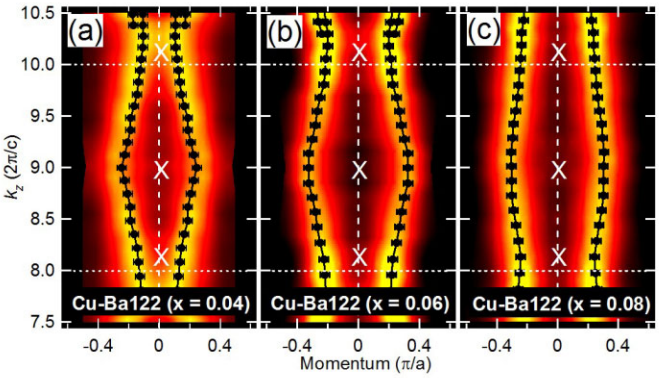

Figure 1: Three dimensionality of FS for nearly optimally doped (a) to overdoped $Ba(Fe_{1-x}Cu_x)_2As_2$ (b, c).

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