Electronic structure of iron-based superconductor $Ba(Fe_{1-x}TM_x)_2As_2$ (*TM* = Ni, Cu) observed by ARPES

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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 almost 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, shift of the 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 the theoretical calculation, it has been reported that the doped *d* electrons 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 result is inconsistent with rigid-band picture observed in the previous ARPES result [5].

In this study, we have studied the electronic structure of $Ba(Fe_{1-x}Ni_x)_2As_2$ and $Ba(Fe_{1-x}Cu_x)_2As_2$ with Ni concentration x = 0.0375, 0.05, and 0.08, and with Cu concentration x = 0.06 and 0.08. Particularly, we focused on the photon energy dependence of ARPES spectra. Figure 1 shows the result of the Fermi surface mapping of the hole and electron FSs for the optimally doped $Ba(Fe_{0.95}Ni_{0.05})_2As_2$ taken at T = 9 K. We find that the hole FS along the Γ-Z direction disappears as a result of the electron doping. In order to estimate hole and electron carrier concentrations of Ni- and Cu-doped $BaFe_2As_2$, the carriers have been counted by Fermi-surface volume for hole and electron FSs. We have also performed FS mapping within k_x - k_y momentum space to discuss the nesting properties in this electron-doped system.

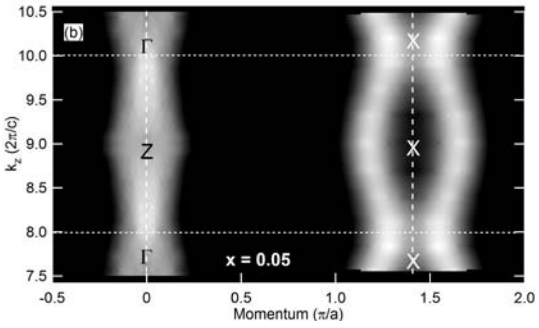

Figure 1: Three dimensionality of FS of optimally doped $Ba(Fe_{1-x}Ni_x)_2As_2$.

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