



Angle-resolved photoemission study of heavily electron-doped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$

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ABSTRACT

We report results of angle-resolved photoemission spectroscopy on a heavily electron-doped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$. By using synchrotron-radiation light, we have investigated the band dispersion near the Fermi level (E_F) of $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ ($x = 0.3$) for different wave vectors perpendicular to the crystal surface (k_z). We find that observed holelike band does not cross E_F around Γ or Z point of the Brillouin zone, unlike the optimally- or under-doped samples. The holelike band also shows a finite k_z dispersion of about 20 meV. These results indicate that the coexistence of hole and electron pockets connected by the antiferromagnetic wave vector plays an important role to the mechanism of superconductivity.

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1. Introduction

The discovery of superconductivity in iron-based superconductors [1] has attracted considerable interest because of their high transition temperatures. In iron-based superconductors, doping of carriers into the antiferromagnetic (AF) parent compounds gives rise to superconductivity. In AFe_2As_2 , the so called 122 system, holes are doped by the chemical substitution of A^{2+} ions by potassium ions (K^+) [2], whereas electrons are doped by replacement of iron atoms with cobalt (Co) or nickel (Ni) ions [3]. So far, angle-resolved photoemission spectroscopy (ARPES) measurements on the hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ has been carried out to reveal the nature of Fermi-surface (FS)-dependent superconducting (SC) gap [4]. On the other hand, few such experiment has been done in the electron-doped counterpart. Upon electron doping, the T_c value of $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ shows a maximum of 25.5 K around $x = 0.15$, and finally vanishes at $x \sim 0.3$ [5]. Clarifying the microscopic origin of such a characteristic phase diagram would be essential in fully understanding the SC mechanism of iron-based superconductors. Previous ARPES study of heavily electron-doped $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$

($x = 0.3$) with the He discharge lamp have clarified that the holelike FS centered at the Γ point, as seen in the hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, is absent or very small while the volume of electron-like FSs significantly expands due to electron doping [6], proposing that the FS nesting between the hole and electron pockets is essential in understanding the mechanism of superconductivity. More recent synchrotron-radiation-based ARPES studies of $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ at the lower doping region have reported that the band structure and the FS have a sizable three dimensionality [7,8], requesting the re-examination of the FS nesting scenario. It is thus particularly important to check the possible three dimensionality of the electronic structure in the heavily overdoped region to finally establish the importance of interband scattering to the mechanism of superconductivity.

In this paper, we report ARPES measurement on heavily electron-doped 122 system by using the synchrotron-radiation light. We have investigated band dispersion for different k_z value and found small k_z dispersion of the holelike band at the zone center. We have also found that the nesting condition is ill defined in this heavily overdoped sample, supporting the conclusion of the previous ARPES experiment with the He lamp.

2. Materials and methods

The high quality single crystals of $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ were grown by the self-flux method [9]. ARPES measurements were performed

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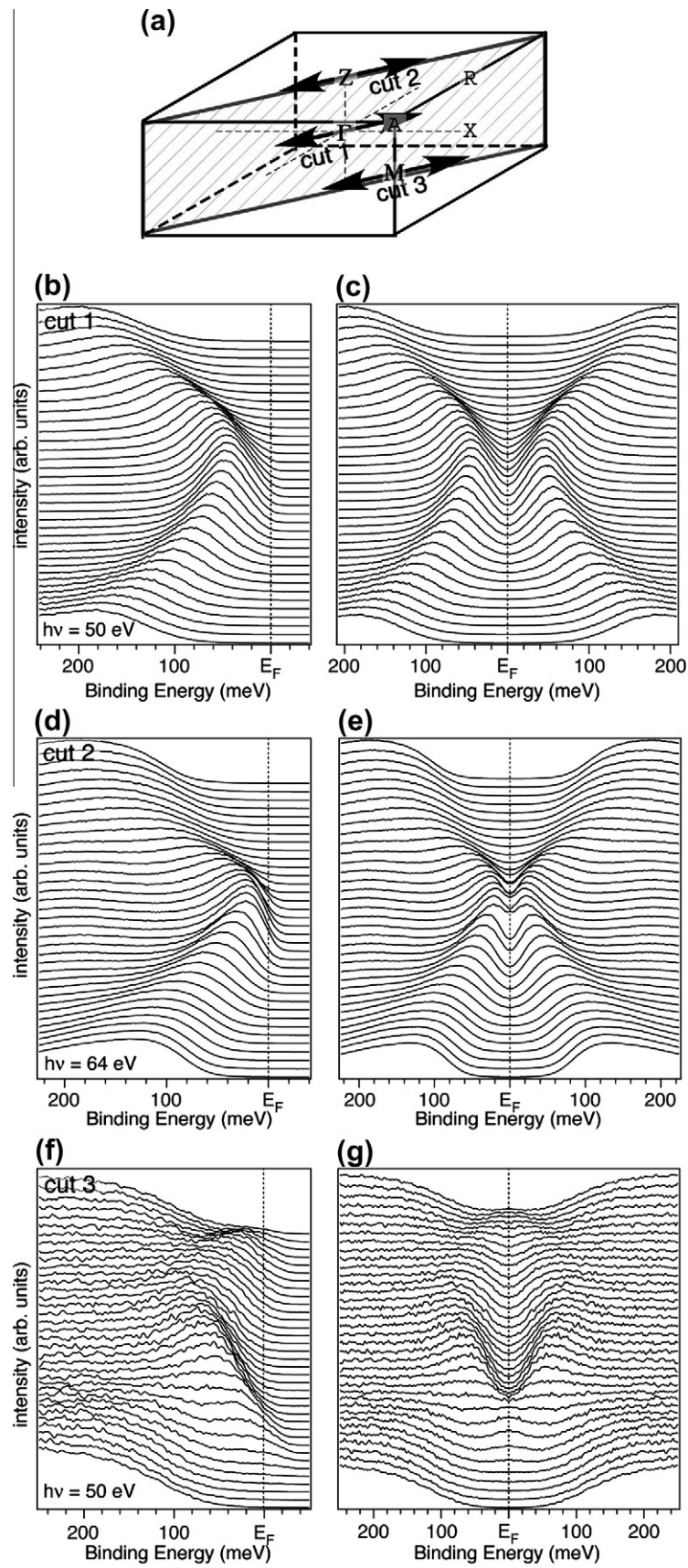


Fig. 1. (a) Schematic view of 3D Brillouin zone and the measured cuts 1–3 (arrows). (b) ARPES spectra at 20 K measured along the cut 1. (c) Symmetrised ARPES spectra of (b). (d) and (e): Same as (b) and (c) but measured at cut 2. (f) and (g): Same as (b) and (c) but measured at cut 3.

using a VG-SCIENTA SES2002 spectrometer at a beamline 28A of photon factory (PF), KEK, Tsukuba. Clean sample surface for the ARPES measurement has been obtained by cleaving *in situ* in an ultrahigh vacuum better than 5×10^{-8} Pa.

3. Results and discussion

Fig. 1b displays the ARPES spectra of $\text{BaFe}_{1.7}\text{Co}_{0.3}\text{As}_2$ ($T_c = 0$ K) in the vicinity of E_F measured at $h\nu = 50$ eV which corresponds to the momentum cut crossing the Γ point as shown in an arrow in (a). We determined the k_z value by the normal emission ARPES measurement (not shown). As clearly seen, we find highly dispersive holelike band centered at the Γ point which does not cross E_F but has a top of dispersion at ~ 50 meV. This non- E_F -crossing behavior is more clearly visualized in the symmetrized spectra shown in (c). As shown in Fig. 1d, the overall band dispersion along cut 2 which cross the Z point is similar to that along cut 1, but the energy position of the band at the Z point is about 30 meV, slightly closer to E_F . Again, this band does not cross E_F as shown in (e). We have confirmed by a detailed photon-energy-dependent measurement that the observed holelike band at the Γ point does not cross E_F in any k_z points, and has a dispersion of ~ 20 meV along k_z . It is noted that we find electronlike FS centered at M point, quite similar to the previous ARPES experiment with the He lamp [6], as shown in Fig. 1f and g. These experimental results suggest that the nesting condition is ill defined in this heavily overdoped sample even when we take into account the three dimensionality of the band structure.

4. Conclusions

In summary, we have reported synchrotron-radiation-based ARPES results of $\text{BaFe}_{1.7}\text{Co}_{0.3}\text{As}_2$. The hole pocket was not clearly observed at the zone center irrespective of the k_z value, resulting in the suppression of the interband scattering through the electron pocket at the M point. This is likely responsible for the disappearance of T_c .

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