The discovery of superconductivity at 26 K \(^1\) (43 K under high pressure \(^2\)) in LaFeAsO\(_{1-x}\)F\(_x\), has triggered intensive researches on the high-temperature (\(T_c\)) superconductivity of iron (Fe) pnictides. The \(T_c\) value has already exceeded 55 K by replacing La atom with other rare-earth atoms or by introducing oxygen vacancies\(^3,4\), opening a new avenue for high-\(T_c\) superconductors are (i) electrons in the Fe orbitals, generally believed to be the foe, indeed play an essential role in superconductivity\(^1,5,6\), (ii) non-doped parent compounds commonly exhibit a collinear antiferomagnetic (AF) spin density wave (SDW)\(^7,8\), and (iii) the superconductivity emerges either by the hole or electron doping into the parent compounds\(^1,9\). To elucidate the mechanism of high-\(T_c\) superconductivity in terms of the electronic structure, angle-resolved photoemission spectroscopy (ARPES) has been performed on both hole- and electron-doped compounds in the optimally- and non(under)-doped region\(^6,10,11,12,13,14,15,16,17\) and it clarified key features on the band structure, the FS topology, and the superconducting gap. On the other hand, little is known about the electronic states in the overdoped region. As demonstrated by electrical resistivity measurements, the \(T_c\) value of the hole-doped Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) monotonically decreases from the optimally-doped region (\(T_c = 37 \text{ K}\)) upon hole doping but does not completely disappear even at the highest doping level \((x = 1.0; T_c \sim 3 \text{ K})\)\(^18,19\), unlike the overdoped cuprates. The resistivity does not show SDW-related anomalies in the overdoped region\(^19\). Clarifying the microscopic origin of this \(T_c\) reduction would be a key to find an essential ingredient to achieve high-\(T_c\) values in the iron-based superconductors. It is thus of particular importance to gain insight into the band structure and the FS by performing ARPES measurements on overdoped samples and directly compare the electronic states with the optimally-doped ones for a comprehensive understanding of the high-\(T_c\) mechanism.

In this Letter, we report high-resolution ARPES results on KFe\(_2\)As\(_2\) (\(T_c = 3 \text{ K}\)), the overdoped limit of Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\) \((A = \text{Alkali earth metal}; x = 1)\). We have determined the band structure near \(E_F\) and the FS topology, and compared with the results of optimally-doped Ba\(_{0.6}\)K\(_{0.4}\)Fe\(_2\)As\(_2\) (\(T_c = 37 \text{ K}\)). We demonstrate that, unlike Ba\(_{0.6}\)K\(_{0.4}\)Fe\(_2\)As\(_2\), the nesting condition via the AF wave vector is not satisfied in KFe\(_2\)As\(_2\). We discuss the implications of the present results in terms of electron correlations and interband scattering.

High-quality single crystals of KFe\(_2\)As\(_2\) used in this study were grown by the flux method\(^20\). High-resolution ARPES measurements were performed using a VG-SCIENTA SES2002 spectrometer with a high-flux discharge lamp and a toroidal grating monochromator. We used the He I\(^\alpha\) resonance line \((h\nu = 21.218 \text{ eV})\) to excite photoelectrons. The energy and angular (momentum) resolutions were set at 4-10 meV and 0.2° (0.007Å\(^{-1}\)), respectively. Clean surfaces for ARPES measurements were obtained by in-situ cleaving of crystals in a working vacuum better than 5×10\(^{-11}\) Torr. The Fermi level \((E_F)\) of the samples was referenced to that of a gold film evaporated onto the sample substrate. Mirror-like sample surfaces were found to be stable without obvious degradation for the measurement period of 3 days. Figure 1 shows ARPES spectra of KFe\(_2\)As\(_2\) measured at 15 K with the He I\(^\alpha\) line along two high-symmetry

Band Structure and Fermi Surface of an Extremely Overdoped Iron-Based Superconductor KFe\(_2\)As\(_2\)
The calculated bands for BaF$_2$ agree with the renormalized LDA calculations. Experimentally determined band structure shows an over-factor of 2. As clearly seen in Figs. 1(c) and (d), the energy on approaching the M point. To see more clearly a broad feature rapidly dispersing toward higher binding energy, we have mapped the ARPES intensity as a function of wave vector and binding energy and show the results in Figs. 1(c) and (d) for the ΓX and ΓM high-symmetry lines (a) ΓX and (b) ΓM. W e also plot the band structure shows a holelike dispersion with respect to the ΓM line.

Especially, a highly-dispersive band in Fig. 1(d) whose energy exceeds 0.5 eV at midway between the Γ and M points is well reproduced by the renormalized calculations. We also find some differences in the energy position of bands between the experiment and the calculations, e.g., the higher-energy bands at the Γ point (0.1-0.2 eV in the experiment vs. 0.2-0.4 eV in the calculations), suggesting that some bands are more strongly renormalized with a renormalization factor of ~4. This implies a possible orbital/momentum dependence of the electron correlation effect.

Figure 2(a) shows the ARPES-intensity plot at $E_F$ as a function of the two-dimensional wave vector measured at 15 K. Bright areas correspond to the experimentally-determined FS. We identify two holelike FSs centered at the Γ point, where the inner one displays a stronger intensity. These FSs are also observed in BaFe$_2$As$_2$ and therefore ascribed to the α (inner) and β (outer) hole pockets. We also find small bright spots slightly away from the M point, called here the ϵ pockets. To clarify the topology of the ϵ FS, we plot in Fig. 2(b) the ARPES intensity in the vicinity of $E_F$ as a function of the wave vector and binding energy for representative cuts (1-6). As seen in the cuts 3-6, the band to produce the ϵ FS is less dispersive than the α and β bands near the Γ point (cuts 1 and 2, respectively) and shows a holelike dispersion with respect to the ΓM line (black dashed line). This ϵ band crosses $E_F$ in cuts 4 and 5, producing a small hole pocket. No evidence for the two electron pockets (γ and δ FSs) has been found at the M point, likely due to the excess of hole doping which lifts the band bottom of the electron pockets above $E_F$.

Figure 3(a) displays a direct comparison of the momentum location of $k_F$ points between the K0.4 and K1.0 samples. As clearly visible, the volume of the α and β...
The measured binding energy of the K₀.₄ sample is shifted downward with respect to that of the K₁.₀ sample, indicating the bulk nature of this measurement. We further speculate that the interband scattering between the α and γ bands is an essential ingredient to achieve high- Tₑ values in iron-based superconductors. We further speculate that the β FS may not contribute deeply to the pairing mechanism in the hole-doped region since its topology and shape are quite similar between optimally- and overdoped samples whereas the Tₑ values are dramatically different. The opening of a small superconducting gap of the β band of the K₀.₄ sample might be due to a proximity effect.

The band calculations (~120 meV), possibly due to the strong mass renormalization of the near-Eₚ bands as seen in Fig. 1. Since the bottom of the electron-like γ band for x = 0.₄ is 18 meV below Eₚ, the γ band for x = 1.₀ completely disappears in the unoccupied region by the observed chemical potential shift of 20-25 meV.

Now we discuss the present ARPES results and their implication on the pairing mechanism. As seen in the schematic band structure in Fig. 4(a), the α and γ FSs of the optimally-doped K₀.₄ sample are well connected by the AF wave vector Q_AF between the hole and electron bands (the α and γ bands) centered at Γ and M points, respectively. The interband scattering is markedly suppressed in the overdoped region due to the absence of the electron FSs at M.

In conclusion, we reported ARPES results on KFe₂As₂ (Tₑ = 3 K) and determined the band dispersion near Eₚ and the FS topology. The experimentally determined FS consists of three types of hole pockets, two centered at the Γ point (α and β), and one around the M point (γ). The small γ electron pocket seen in the optimally-doped...
sample is completely absent, resulting in the suppression of the $Q_{AF} = (\pi, \pi)$ interband scattering which is likely responsible for the reduction of $T_c$ values in the overdoped region.

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