Angle integrated photoemission study of SmO$_{0.85}$F$_{0.15}$FeAs

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The electronic structure of the new superconductor, SmO$_{1-x}$F$_x$FeAs ($x = 0.15$), has been studied by angle-integrated photoemission spectroscopy. Our data show a sharp feature very close to the Fermi energy, and a relative flat distribution of the density of states between 0.5 eV and 3 eV binding energy, which agrees best with band structure calculations considering an antiferromagnetic ground state. No noticeable gap opening was observed at 12 Kelvin below the superconducting transition temperature, indicating the existence of large ungapped regions in the Brillouin zone.

The discovery of superconductivity with an unexpectedly high superconducting transition temperature ($T_c$) of 26K in the iron-based LaO$_{1-x}$F$_x$FeAs ($x = 0.05 - 0.12$) has ignited intensive studies recently$^{[1]}$. Particularly, Chen et al. has raised the $T_c$ to 43 K with SmO$_{1-x}$F$_x$FeAs ($x = 0.15$)$^{[2]}$, a record high for non-cuprate superconductors. Such a high $T_c$ is hard to understand within the conventional BCS mechanism for superconductivity$^{[3]}$. Up to now, multiple pieces of evidences have been gathered in recent studies to unveil the nature of these novel superconductors. Experiments from the specific heat measurements$^{[4]}$, point-contact tunneling spectroscopy$^{[5]}$, and infrared reflectance spectroscopy$^{[6]}$ provided support of the existence of unconventional superconductivity in such materials.

The band structure of LaO$_{1-x}$F$_x$FeAs has been calculated by density functional theory (DFT) and dynamical mean field theory (DMFT), based on which various theoretical proposals have been put forward. For example, it has been revealed that the electron-phonon interaction in the system is too small to support such high $T_c$'s$^{[7]}$, while various unconventional superconducting pairing symmetries have been proposed$^{[8, 9, 10]}$. Considering the possible strong correlation involved, these results remain to be verified experimentally. However, besides a few pieces of transport measurements on polycrystalline samples, no direct measurement of the electronic structure has been reported so far.

In this paper, we report angle integrated photoemission spectroscopy measurement of a SmO$_{0.85}$F$_{0.15}$FeAs polycrystal, which gives the density of states (DOS) of the system. A relatively narrow feature at 0.25 eV was observed, which agrees very well with DFT calculations based on an antiferromagnetic ground state. No noticeable gap opening was observed even at 12 Kelvin below the superconducting transition temperature, indicating the existence of large ungapped regions in the Brillouin zone. Our data put strong constraints on theoretical studies.

![FIG. 1: Angle integrated spectrum of SmO$_{1-x}$F$_x$FeAs (a) over a large energy window, and (b) within the shaded region of (a). Data in (a) and (b) were taken at 45K with 40.8eV and 21.2eV photons correspondingly.](image)
formed with Helium-I $\alpha$ (21.2 eV) and Helium-II (40.8 eV) emission lines of a Helium discharge lamp. Data were taken with a Scienta R4000 electron analyzer. The energy resolution is 10 meV. The sample rod was broken \textit{in-situ} and then measured in ultra-high vacuum ($\sim 3 \times 10^{-11}$ mbar). The isotropic distribution of the polycrystal orientation was confirmed by varying the photoelectron emission angle.

The angle integrated spectrum of SmO$_{0.85}$F$_{0.15}$FeAs shown in Fig.1(a-b) measures the DOS of the system. Except the low energy feature near the Fermi energy ($E_F$), it is quite flat within the first 3 eV below $E_F$, and stronger features only show up from 3 eV binding energy and higher. The low energy feature was attributed to Fe 3$d$ states in various DFT band structure calculations \cite{1,4,5,6,7,8,9,10}. However, there are quantitative differences amongst them. Our data, especially the peak at 0.25 eV and the flat distribution between 0.5 eV to 3 eV binding energy, agree best with the DFT calculation that considers an antiferromagnetic ground state \cite{13,14}. On the other hand, this low energy feature does not show up in dynamical mean field theory calculation \cite{15}.

In order to study the superconducting gap, the angle-integrated spectrum near $E_F$ is taken as a function of temperature (Fig.2a). There is a clear cutoff by the Fermi function, and the middle point of the leading edge crosses the Fermi energy for all spectra. Fig.2b compares the 31K spectrum with 42K spectrum after removing the thermal broadening effects due to their temperature difference (details in caption). It seems they overlap very well. For an s-wave superconductor, at a temperature of 75\% $T_c$, more than 60\% of the gap would have already opened. The absence of any sign of gap-opening in the DOS measured here might be partially attributed to the broad transition in this polycrystalline sample. Nevertheless it does indicate that large portions of the Fermi surface are still ungapped at 12 K below $T_c$ for SmO$_{0.85}$F$_{0.15}$FeAs, which is a sign of unconventional superconductivity. Future measurements on high quality single crystal are necessary to further clarify this issue. Moreover, we note that an anomaly at about 150K was observed in the resistivity data \cite{2}, which resembles the pseudogap effects in cuprate superconductors. However, our data taken above and below 150K did not show any sign of pseudogap opening.

To summarize, we have reported angle-integrated photoemission spectroscopy results of the new superconductor SmO$_{0.85}$F$_{0.15}$FeAs. Our data, particularly the sharp feature at 0.25 eV below the Fermi energy, put quite strong constraints on various theoretical calculations. No appreciable gap effects on the density of states were observed at 12 Kelvin below the superconducting transition temperature, indicating possible existence of large ungapped regions in the Brillouin zone.

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[17] We note that although Sm replaces La here, they both would contribute negligibly to the shallow band structure. Therefore, one can compare our data with the band structure calculation of LaO$_{1-x}$F$_x$FeAs.