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Doping dependence of electron correlation in FeTe$_{1-x}$Se$_x$ studied by angle-resolved and resonance photoemission spectroscopy

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1 Introduction

FeTe is expected to have the strongest electron correlation among the iron-based superconductors and the electron correlation may show strong orbital dependence [1,2]. FeSe on the other hand is expected to show only moderate electron correlation and its orbital dependence comparable to other iron-based superconductors [1]. Alloying FeTe with FeSe may give us insight on how the electron correlation and the orbital dependence change with doping. To investigate this issue, we have performed resonance and angle-resolved photoemission spectroscopy (ARPES) experiments on FeTe$_{1-x}$Se$_x$ (x = 0, 0.4, 1).

2 Experiment

Samples were synthesized using the Bridgman method. Only polycrystals were synthesized for FeSe samples while single crystals were obtained for the rest of the compositions. Angle-resolved and resonance photoemission measurements were performed at beam line 28A of Photon Factory, KEK using circularly polarized light of *hν*= 80 eV. The samples were cleaved *in situ* under the base pressure of better than 9 x 10^{-9} Pa.

3 Results and Discussion

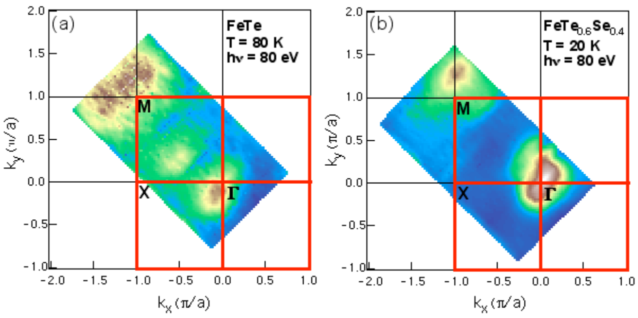

Fig. 1: Photoemission intensity distribution integrated over the energy window E_F – 10 meV < E_F + 10 meV for (a) FeTe and (b) FeTe$_{0.6}$Se$_{0.4}$ as a function of the two-dimensional wave vector taken at 80 K and 20 K, respectively with 80 eV photons. The red line marks the boundary of the first Brillouin zone.

Figure 1 shows the momentum distribution of photoemission intensity for (a) FeTe and (b) FeTe$_{0.6}$Se$_{0.4}$ at the Fermi energy. The data were taken at 80 K and 20 K, respectively with 80 eV photons. Similar to other iron-based superconductors, the spectral weight around Γ and M points is mostly located in the near-E_F region. The spectra are characterized by a broad feature, which is suggested to be due to strong electron correlation in this compound [3].

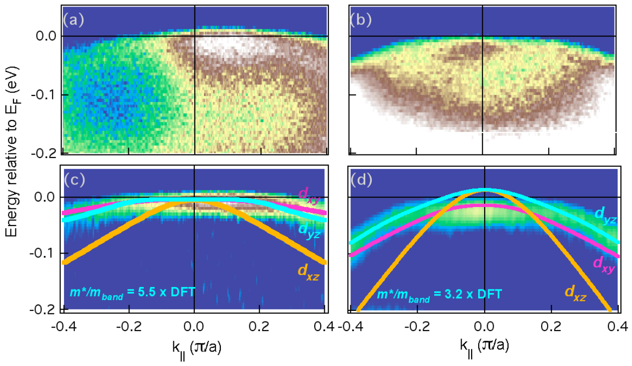

Fig. 2: (a),(b) Intensity plot near E_F for FeTe and FeTe$_{0.6}$Se$_{0.4}$, respectively. (c),(d) Second-derivative plot of momentum distribution curves (MDCs) for FeTe and FeTe$_{0.6}$Se$_{0.4}$, respectively, together with the calculated band dispersions [4].

Shown in Fig. 2(a) and 2(b) are the ARPES intensity in the near-E_F region for FeTe and FeTe$_{0.6}$Se$_{0.4}$, respectively. Near the Fermi level, two band dispersions with d_{yz} and d_{xz} orbital characters are observed around the Γ point. Features near E_F qualitatively agree with the calculated band structure after being reduced along the energy direction by a renormalization factor. The renormalization factor is found to be orbital dependent with the d_{yz}-orbital band more strongly renormalized than the d_{xz}-orbital band. For FeTe$_{0.6}$Se$_{0.4}$, the mass renormalization factors for d_{yz} and d_{xz} are 3.2 and 2, respectively. Note that the d_{xz} orbital contributes a nearly straight dispersing feature and thus cannot be recognized from the energy distribution curves (EDCs) (not shown here) as well as on the second-derivative of EDCs. Only the d_{yz}-orbital band is clearly seen in the second-derivative plot of EDCs shown in Figs. 2(c) and 2(d) for FeTe and FeTe$_{0.6}$Se$_{0.4}$, respectively. In addition to the orbital dependence of the mass renormalization, it is also doping dependent. The mass renormalization factor for d_{yz}

for FeTe is about 5.5, which is larger than in $FeTe_{0.6}Se_{0.4}$. This result suggests that the substitution of Se into FeTe weakens the strength of electron correlation as exhibited by the decrease of the mass renormalization factor for the d_{yz} orbital band.

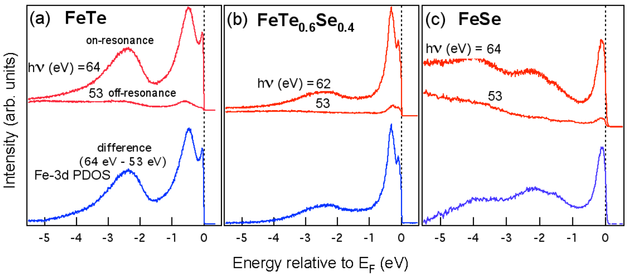

Fig. 3: Fe 3*d* PDOS of (a) FeTe, (b) $FeTe_{0.6}Se_{0.4}$, and (c) FeSe determined by subtracting the off-resonance from the on-resonance spectra.

At the binding energy of about 0.3 – 1 eV (not shown here), dz^2 orbital band can also be observed, at least for FeTe. The dz^2 orbital band is renormalized with a factor of 1.8, which also shows the orbital-dependence of the mass renormalization and that deep bands are weakly correlated when compared to the bands near the Fermi level. However for $FeTe_{0.6}Se_{0.4}$, deeper binding energy bands is not clearly observed. To further clarify the renormalization effect on the dz^2 orbital, we have performed resonance photoemission spectroscopy. Figure 3 shows the Fe-3*d* partial density of states (PDOS) of (a) FeTe, (b) $FeTe_{0.6}Se_{0.4}$ and (c) FeSe. The partial density of states (PDOS) for the Fe-3*d* electrons is taken from the difference between the on-resonance and off-resonance valence band spectra. Near the Fermi level, a region up to ~ -1 eV, two distinct features can be clearly seen in FeTe and $FeTe_{0.6}Se_{0.4}$ while only one merged structure can be observed in FeSe. The energy position of the strongest peak shifts towards the Fermi level with increasing Se concentration. The shift of the peak position with Se substitution is qualitatively consistent with the ARPES result and the DFT calculation [4]. This peak structure can then be attributed mainly to the dz^2 orbital band. The dz^2 orbital band is expected to be weakly correlated but in order to determine the quantitative value of the correlation and its doping dependence, careful analysis, like the phenomenological self-energy correction, should be done.

In conclusion, we have investigated the electron correlation of $FeTe_{1-x}Se_x$ (x = 0, 0.4, 1) by resonance and angle-resolved photoemission spectroscopy (ARPES). The mass renormalization is indeed orbital and doping dependent consistent with the DMFT calculation [1].

References
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