

ЭЛЕКТРОННЫЕ СТРУКТУРА И СВОЙСТВА

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Temperature Evolution of Charge Carrier Density in the Centre of the Brillouin Zone of Fe(Se,Te) Superconductor

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A characteristic feature of the electronic structure of iron-based superconductors is the shift of experimental electronic bands in comparison to the results of calculations. The temperature dependence of the band structure for FeSe can manifest the mechanism of such shifts, but different studies give opposite directions for these shifts in the centre of the Brillouin zone. In this paper, we report downward shift of both d_{xz} and d_{yz} bands in Z point within the temperature range 20–160 K. Together with the results of evolution of

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the electronic structure in A point, such shifts should lead to a break of parity between electron and hole charge carriers that can be interpreted as an increase of electron-carrier density with increasing temperature.

Key words: angle resolved photoemission spectroscopy (ARPES), curvature method, electronic structure, iron-based superconductors, FeSe.

Характерною особливістю електронної структури надпровідників на основі заліза є зсув експериментально одержаних зон порівняно з результатами розрахунків. Зміни електронної структури FeSe з підвищенням температури можуть пояснити механізми таких зсувів, але результати різних досліджень дають протилежні напрямки еволюції зонної структури у центрі Бріллюєнової зони. У цій статті ми повідомляємо про синхронний зсув d_{xz} - та d_{yz} -зон у точці Z у температурному діапазоні 20–160 К. Із врахуванням результатів змін зонної структури з температурою у точці A такі зсуви можуть змінити паритет між електронами та дірками, що може інтерпретуватись як підвищення густини електронних носіїв з підвищенням температури.

Ключові слова: електронна спектроскопія з кутовою роздільною здатністю, метод кривини, електронна структура, залізни надпровідники, FeSe.

Характерной особенностью электронной структуры сверхпроводников на основе железа является смещение экспериментально полученных зон по сравнению с результатами расчётов. Изменения зонной структуры FeSe с повышением температуры могут объяснить механизмы таких смещений, но результаты разных исследований дают противоположные направления эволюции зонной структуры в центре зоны Бриллюэна. В этой статье мы сообщаем о синхронном смещении d_{xz} - и d_{yz} -зон при повышении температуры в точке Z в температурном диапазоне 20–160 К. С учётом результатов изменений зонной структуры с повышением температуры в точке A такие смещения могут изменять паритет между электронами и дырками, что можно интерпретировать как увеличение концентрации электронов с увеличением температуры.

Ключевые слова: фотоэлектронная спектроскопия с угловым разрешением, метод кривизны, электронная структура, железные сверхпроводники, FeSe.

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1. INTRODUCTION

FeSe is one of the most interesting compounds among iron-based superconductors due to interesting physical properties and simplicity of its crystal structure [1–4]. FeSe is a compensated metal with equal numbers of holes and electrons, and its calculated electronic structure, similarly to other iron-based superconductors, consists of 2 holes-like bands near the Fermi level in the centre of the Brillouin zone (Gamma

point) and 2 electrons-like bands in its corners (M -point), which come from $3d$ bands of iron. Such topology have been predicted by numerous density functional theory (DFT) calculations [5, 6] and confirmed by many experiments [7, 8]. However, there are some differences between results of calculations and experimentally obtained data.

First, it is a mass enhancement of charge carriers, which is supposed to be a result of electron correlations and can be explained by dynamical mean-field theory (DMFT) calculations [9–12].

Another difference is a shrinking of experimentally obtained Fermi surfaces in comparison to DFT calculated ones. Such a shrinking is supposed to be a result of the shifts of bunches of the hole and electron bands in the opposite directions, with conservation of parity between electrons and holes [4, 13, 14]. Namely, the hole bands in the Brillouin zone centre shift to higher binding energies, and electron bands in M point (the Brillouin zone corners) to lower binding energies. Such shifts cannot be obtained within the DMFT calculation framework even for the simplest iron based superconductor FeSe.

Recent works propose several mechanisms that can explain such shifts [4, 15–18]. To examine applicability of such mechanisms, the investigations of the temperature dependence of the band structure of FeSe compounds have been performed [18–20]. Interestingly, the results of different investigations give opposite directions for the temperature-induced shifts in Z point.

In previous paper [20], it has been shown that the d_{yz} band moves in opposite direction to the ‘red-blue’ shift expectation and to some recent results [19], but agrees with another experimental data [18]. The shift of this band cannot affect the size of the hole-like Fermi surface, as the d_{yz} band does not cross the Fermi level. In this paper, we reveal downward shift of the d_{xz} and d_{yz} bands in Z point of FeSe. The shift of the d_{xz} band causes shrinking of the hole-like Fermi surface in the Brillouin zone centre. In terms of charge carrier concentration, together with the results of temperature dependence in A point, such shifts can be interpreted as appearance of additional electrons in the system.

2. EXPERIMENTAL DETAILS

ARPES spectra have been obtained on CASIOPEE beamline of synchrotron Soleil using horizontally polarized radiation with energy 21 eV, for temperatures 20 K, 100 K, and 160 K. Experimental ARPES spectra for 20 K, 100 K, and 160 K and the results of processing of spectra with two-dimensional curvature method are presented in Figs. 1–3, respectively. The hole bands’ top position for different temperatures was obtained by image processing with two-dimensional curvature method and are given in Fig. 4.

The crystals $\text{Fe}_{1.05}\text{Se}_{0.84}\text{Te}_{0.16}$ have been grown in evacuated quartz

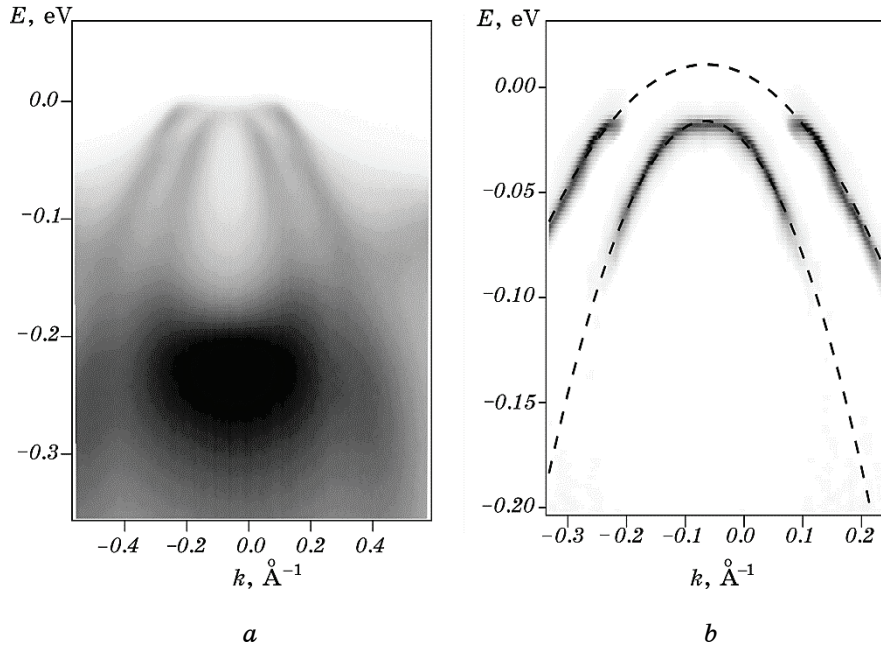


Fig. 1. ARPES spectrum for 20 K (a) and the results of processing of the spectrum with the curvature method (b).

ampoules using the AlCl_3 – KCl – NaCl flux technique with a constant temperature gradient (500°C —temperature of the hot end, $\sim 430^\circ\text{C}$ —temperature of the cold end, $\text{Fe}_{1.3}\text{Se}_{0.8}\text{Te}_{0.2}$ —composition of the start load, 6 weeks) [21]. The chemical composition of the $\text{Fe}(\text{Se},\text{Te})$ crystals was determined using a Tescan Vega II XMU scanning electron microscope equipped with an INCA Energy 450 energy-dispersive spectrometer (accelerating voltage—20 kV).

3. RESULTS AND DISCUSSION

ARPES spectra have been obtained for temperature 20 K (lower than the nematic transition), 100 K (higher but in vicinity to the nematic transition) and for 160 K.

In case of linear horizontal polarization, both the hole-like d_{xz} and d_{yz} bands can be seen near the Fermi level. It is in contrast to the results of the linear vertical polarization, where only one hole d_{yz} band can be seen due to matrix element effects. The temperature dependence obtained earlier in [20] for d_{yz} band is confirmed by these results. Important to mention that the d_{yz} band does not cross the Fermi level. Therefore, temperature induced shift of this band cannot affect the number of charge carriers. So, it is important to track dependence of

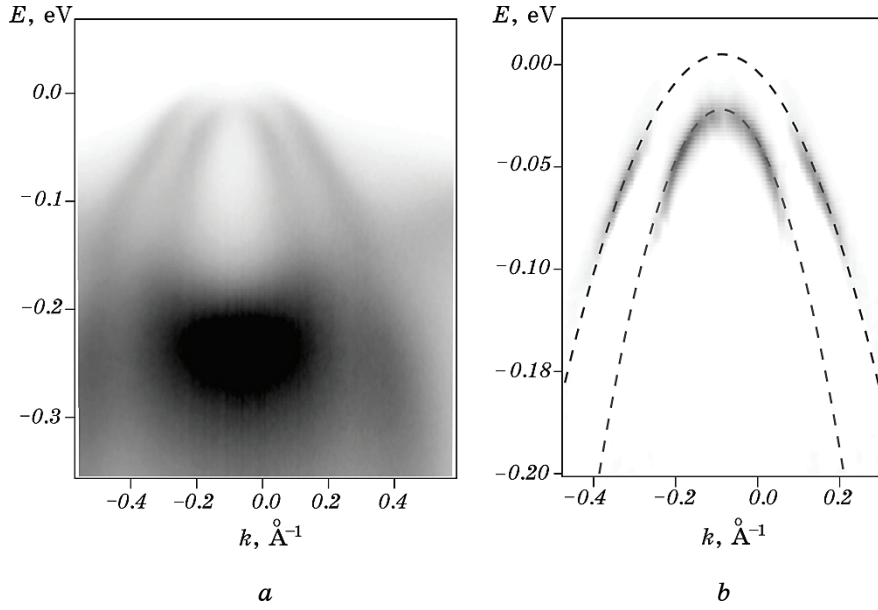


Fig. 2. ARPES spectrum for 100 K (a) and the results of processing of the spectrum with the curvature method (b).

the d_{xz} band on temperature, because it crosses the Fermi level. The shift of this band strongly affects the size of the hole Fermi surface. It is important to say that, in opposite to [7, 8], we do not observe the splitting of the d_{xz} band for temperatures lower than the temperature of nematic transition near the Fermi level.

The energies of the tops of the d_{xz} and d_{yz} bands for different temperatures that have been obtained from the spectra are given in Fig. 4. Several important features of this dependence should be mentioned. First, binding energy of electrons increases with increase of temperature for both bands. Second, since there is no additional splitting between the hole-like bands in temperature range from 20 to 160 K, we may conclude that the observed shift is a characteristic feature of the whole electronic structure in Z point.

Other studies give different directions of temperature shifts of the band structure in Z point, but there is a consensus in determination of the direction of band structure evolution in A point [18, 19]. In both studies, the electron-like bands in the Brillouin zone corner move downwards in energies. So, the area of the electron-like Fermi surfaces becomes larger. The shrinking of the hole-like Fermi surface in Z point and the expansion of electron-like of hole-like Fermi surface in A point change the ratio between area of hole and electron surfaces. It is equivalent to change of charge carrier concentration, although there are arguments [14, 18] that these shifts do not imply a change of stoichiome-

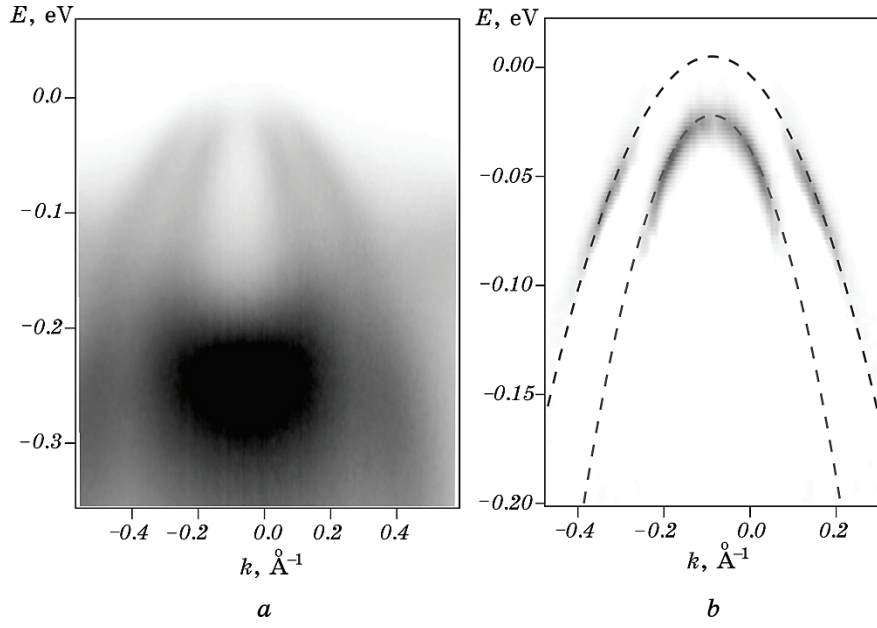


Fig. 3. ARPES spectrum for 160 K (a) and the results of processing of the spectrum with the curvature method (b).

try but are the results of chemical potential shift due to its proximity to the edges of the bands.

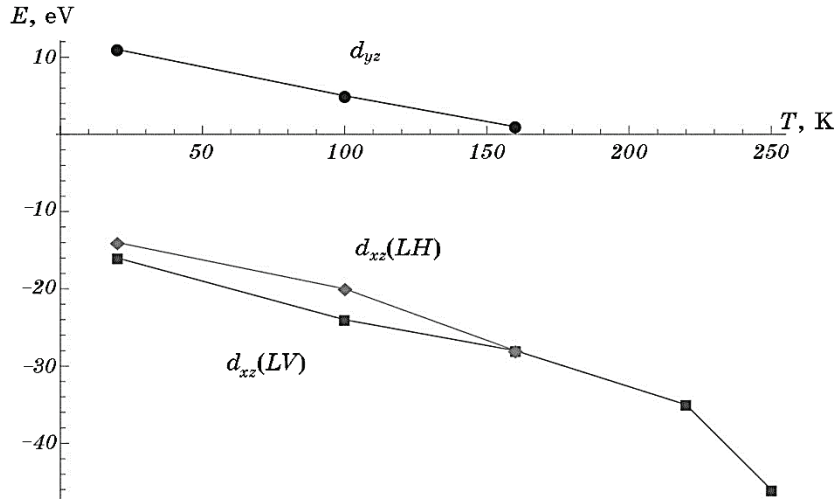


Fig. 4. Positions of the d_{xz} and d_{yz} bands in Z point from the ARPES spectra obtained with horizontal polarization ($d_{yz}(LH)$) and the results for $d_{yz}(LV)$ from [20].

4. CONCLUSIONS

Using photons with horizontal polarization, we have shown that the both d_{xz} and d_{yz} hole-like bands in Z point move in the same direction with the same speed, lowering their energy with increasing temperature. This confirms previous result for d_{yz} band shift obtained from the spectra measured with vertical polarization [20] but contradicts to the ‘red-blue shift’ model and to some of recent experiments [19]. Taking into account the expansion of the electron-like Fermi surfaces in the Brillouin zone corner with temperature, our observation implies the temperature induced break of the parity between holes and electrons that should be understood.

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