A flat band at the chemical potential of a Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$ superconductor observed by angle-resolved photoemission spectroscopy

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Received 4 December 2012, in final form 22 March 2013
Published 19 April 2013
Online at stacks.iop.org/JPhysCM/25/195701

Abstract

The electronic structure of superconducting Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$ has been studied by angle-resolved photoemission spectroscopy (ARPES). Experimental band topography is compared to the calculations using the methods of Korringa–Kohn–Rostoker (KKR) with the coherent potential approximation (CPA) and the linearized augmented plane wave with local orbitals (LAPW + LO) method. The region of the $\Gamma$ point exhibits two hole pockets and a quasiparticle peak close to the chemical potential ($\mu$) with undetectable dispersion. This flat band with mainly $d_{\text{z}^2}$ orbital character is most likely formed by the top of the outer hole pocket or is evidence of a third hole band. It may cover up to 3% of the Brillouin zone volume and should give rise to a Van Hove singularity. Studies performed for various photon energies indicate that at least one of the hole pockets has a two-dimensional character. The apparently nondispersing peak at $\mu$ is clearly visible for 40 eV and higher photon energies, due to an effect of the photoionization cross-section rather than band dimensionality. Orbital characters calculated by LAPW + LO for stoichiometric FeTe do not reveal the flat $d_{\text{z}^2}$ band but are in agreement with the experiment for the other dispersions around $\Gamma$ in Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$.

(Some figures may appear in colour only in the online journal)

1. Introduction

The search for new superconducting materials and the opportunity to discover further evidence of non-BCS mechanisms of electron pairing have directed the attention of researchers to iron pnictides [1, 2] and chalcogenides [3–10]. Among these materials the systems from the ‘11’ group, namely Fe$_{1+x}$Se [3], Fe$_{1+x}$Te$_{1-y}$Se$_y$ [11], and Fe$_{1+x}$Te$_{1-y}$S$_y$ [5], have the simplest crystallographic structure with iron atoms arranged in characteristic planes (figure 1). These Fe(1) atoms, tetrahedrally coordinated by chalcogen atoms, form layers separated by van der Waals gaps. In consequence
The ‘11’ systems can be regarded as quasi-two-dimensional. Nevertheless, this structure features an intrinsic disorder due to both excess iron in partially occupied Fe(2) positions [12] and substituted atoms, which are displaced with respect to the Te crystallographic positions. It is known that doped S atoms substitute Te but is displaced along the c crystallographic axis with respect to the Te position [13]. Both Te and S positions are shown.

The superconducting critical temperature for ‘11’ chalcogenides is relatively low under ambient pressure and barely reaches 14 K [11] for Fe$_{1+y}$Te$_{1-x}$Se$_y$, 13 K for FeSe [3] and 10 K for Fe$_{1+y}$Te$_{1-x}$S$_y$ [5], while Fe$_{1.1}$Te remains a non-superconducting antiferromagnet [6]. Moreover, the superconducting fraction of untreated FeTe$_{0.8}$S$_{0.2}$ as determined from magnetic susceptibility is close to 20% [6]. The direct connection between the iron overstoichiometry, magnetism and superconductivity can be exposed by topotactic deintercalation using iodine [14, 15] or other oxidation processes like annealing in oxygen [16, 17]. Samples with the lowest content of excess iron have the highest SC fraction, reaching 100%. The promising fact is that under high pressure the transition to superconductivity reaches $T = 37$ K for FeSe [18, 19].

While the mechanism of electron pairing in the Fe-based superconductors is still under debate, the electronic band structure can impose certain conditions on possible scenarios [2]. Therefore, the Fermi surface (FS) and the electronic band structure of the discussed systems have been extensively studied by means of angle-resolved photoemission spectroscopy (ARPES), quantum oscillations and density functional theory (DFT) calculations [6, 2, 20]. In particular, the previous ARPES studies on ‘11’ chalcogenides covered both non-superconducting Fe$_{1+y}$Te [21–23] and superconducting Fe$_{1+y}$Te$_{1+y}$Se$_y$ [24–28] but corresponding results for FeSe or Fe$_{1+x}$Te$_{1+y}$S$_y$ are so far absent from the literature. While the published data for Fe$_{1+y}$Te$_{1+y}$Se$_y$ are relatively consistent, studies of Fe$_{1+y}$Te present two aspects: on the one hand clearly visible band topography [21], on the other hand intrinsically broad spectra in a paramagnetic state with the emergence of quasiparticle peaks in the spin density wave (SDW) state [22]. The latter scenario is confirmed by a more recent study of Fe$_{1.07}$Te and can be understood in terms of polaron formation [23]. The FS of superconducting Fe$_{1+y}$Te$_{1+y}$Se$_y$ chalcogenides consists of hole pockets located around the $\Gamma(\Delta)$ point and electron pockets in the region of the M(A) point, which is typical of both iron pnictides and chalcogenides. However, the newer $\text{A}_x\text{Fe}_{2-y}\text{Se}_2$ systems ($\text{A} = \text{K}, \text{Cs}, \text{Rb}, \text{Tl}$ etc) are exceptional in that respect as they exhibit electron pockets at the $\Gamma(\Delta)$ point [29–32].

The current paper presents the band structure and dominant orbital characters obtained by ARPES for a Fe$_{1.05}\text{Te}_{0.94}\text{S}_{0.06}$ superconductor. The data are compared to theoretical calculations. A flat band close to the chemical potential ($\mu$) is found in the region of the $\Gamma$ point. The resulting high density of states at $\mu$ should be an important factor for the emergence of superconductivity in the sulfur doped ‘11’ compounds.

### 2. Experimental details

Single crystals with targeted stoichiometry Fe$_{1.1}\text{Te}_{0.875}\text{S}_{0.125}$ were grown in NIST by similar techniques as reported earlier [13]. Stoichiometric quantities of the elements were sealed in evacuated quartz tubes and heated at 775 °C for 48 h with an intermediate step at 450 °C. After regrinding, the product was reheated at 825 °C for 12 h and slowly cooled to room temperature. X-ray diffraction performed at 290 K indicated single crystals with a composition of Fe$_{1.11}\text{Te}_{0.91}\text{S}_{0.12}$ as obtained from the Rietveld refinement to x-ray data. The determined crystal structure, as shown in figure 1, is consistent with the previous studies [13] and remains tetragonal to the lowest temperature $T = 35$ K reached in the experiment. The composition of the single crystals was also determined using a JEOL JXA 8900 microprobe in wavelength dispersive mode (WDS) from 10 flat points spread over the surface. The average composition was found to be Fe$_{1.03(1)}\text{Te}_{0.94(4)}\text{S}_{0.06(2)}$ and will be used in the text as being more reliable than the estimate from the diffraction data. The single crystals exhibited the onset of the superconducting transition at $T = 9$ K in magnetic susceptibility and electrical resistivity. However, according to the magnetic susceptibility studies the Meissner phase at $T = 2$ K covered 23% of the volume.

The ARPES experiments were carried out at the APE beamline [33] of the Elettra synchrotron using a Scienta SES2002 electron spectrometer. The crystals were cleaved at a pressure of $2 \times 10^{-11}$ mbar and studied with linearly or circularly polarized radiation. The energy and wavevector ($k$) resolution were 20 meV and 0.01 Å$^{-1}$ respectively. Low energy electron diffraction was used to check the surface quality. Fermi edge determination was performed regularly on evaporated gold.

Band structure calculations were carried out with the AkaiKKR software [34] based on the Korringa–Kohn–Rostoker (KKR) Green’s function method with the coherent potential approximation (CPA). This method is able to model the effect of disorder in alloys [35, 36] and should treat...
The electronic structure of superconducting Fe\(_1\_03\)Te\(_{0\_94}\)S\(_{0\_06}\) crystals (figure 2(a)) was studied by means of ARPES along the high symmetry directions \(\Gamma\leftarrow M\) and \(\Gamma\leftarrow X\) (figure 2(b)). Radiation of linearly polarized photons with an energy of 40 eV was used. The spectra obtained along the \(\Gamma\leftarrow M\) direction at 80 K (figures 2(c), (d)) exhibit high intensity in the region of the \(\Gamma\) point. For \(\sigma\)-polarization a hole pocket is found, whereas for \(\pi\)-polarization the measurements reveal a hole-like band and a feature with high intensity at \(\mu\). The nature of this high spectral intensity will be discussed further. Photoelectron spectra obtained in the region of \(M\) with \(\sigma\)-polarization reveal increased intensity near \(\mu\) at the \(M\) point. The \(\sigma\)-polarization is more favourable for the bands at \(M\), similarly to the case of undoped FeTe [21]. The spectra recorded with \(\pi\)-polarization do not reveal any bands in this region. Near the \(X\) point no spectral intensity is found at low binding energy (not shown). In particular, a replica of the band structure at \(\Gamma\) is not found at \(X\) in contrast to the observations for undoped Fe\(_{1\_14}\)Te [21]. This indicates that the SDW magnetic order is not seen in the Fe\(_{1\_03}\)Te\(_{0\_94}\)S\(_{0\_06}\) system with ARPES.

KKR-CPA calculations, which are destined for systems with disorder, were performed for Fe\(_{1\_1}\)Te\(_{0\_9}\)S\(_{0\_1}\) (figure 2(e)). Despite slightly higher S content than in the measured samples, the calculations should yield the overall effect of doping. The theoretically obtained spectra are broadened due to disorder, which should be reflected in the ARPES data. LAPW + LO calculations (figure 2(f)) were realized for the stoichiometric FeTe system as this approach cannot deal with fractional atomic site occupancies. There is a qualitative agreement between the band structure obtained with these two methods; in both cases three hole pockets are present at the \(\Gamma\) point, two electron pockets are found at the \(M\) point, while there is no FS around the \(X\) point. The difference is observed at the \(M\) point, where the band seen below \(-0.6\) eV for KKR-CPA is located below \(-1.2\) eV for LAPW + LO results, which is off the scale for the figure 2(f). Differences are also visible for the \(\Gamma\leftarrow Z\) direction. A dispersion along \(\Gamma\leftarrow Z\) is a matter of interest, as it may indicate whether the system is two-dimensional. In fact, weak dispersions or even lack of dispersion for certain bands are observed, which is seen in particular for the KKR-CPA approach. This means that this system may be considered as quasi-two-dimensional to some extent. It is also noteworthy that the dispersions...
Figure 3. Energy bands in the Γ point region for Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$ obtained by ARPES along the M–Γ–M direction with (a) π and (b) σ polarizations and along X–Γ–X, with (c) π, (d) σ, (e) circular plus and (f) circular minus polarizations. The experimental dispersions are named as α, β$_1$ and β$_2$. Theoretical dispersions obtained by KKR-CPA calculations (solid lines) are superimposed on the graphs. The spectra are shown as energy distribution curves (EDCs) in (g)–(l). The spectra from (c) and (d) divided by the Fermi function are presented in (m) and (n) respectively. Experimental band dispersions marked by black points result from energy or momentum distribution curve fitting. The extracted dispersions are compared to KKR-CPA (for Fe$_{1.1}$Te$_{0.9}$S$_{0.1}$) and LAPW + LO (for FeTe) calculations (o). Panel (p) shows extracted EDCs from (c) or (i) and the curve resulting from wavevector (k) integration of all EDCs between −0.1 Å$^{-1}$ and 0.1 Å$^{-1}$ from (c) or (i)—red line (dashed). All measurements were performed with incident photon energy of 40 eV at a temperature of 35 K.

near Γ obtained with KKR-CPA are characterized with lower slopes and higher band masses as compared to LAPW + LO at low binding energies. The discrepancies between the obtained band structures may have arisen from different exchange–correlation potentials and different modelling of atomic spheres in the approaches as well as due to the differences between the objects of the studies: Fe$_{1.1}$Te$_{0.9}$S$_{0.1}$ and FeTe. To obtain agreement between the experiment and the theory the Fermi energy for the calculated band structure needs to be shifted up by 0.11 eV and 0.10 eV for KKR-CPA and LAPW + LO respectively.

The band structure obtained from the calculations is generally consistent with the ARPES results both along the Γ–M and Γ–X directions assuming that certain bands may be invisible in the experiment due to unfavourable matrix elements. Out of the three hole pockets predicted by calculations at least two hole-like bands at Γ are found in the experiment. Theoretical results are also consistent with the spectra near M taken along the Γ–M direction (figure 2(c)), where a band moves towards μ when $k$ approaches M, which is visible for σ-polarization. The calculated electron pocket at M is not resolved in the experiment. Theoretical dispersions along Γ–X confirm the absence of energy bands near μ at X.

3.2. Band structure near the Γ point

Let us analyse the region of the Γ point for Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$, where the band structure appears to be different from that observed before for undoped non-superconducting Fe$_{1.4}$Te [21–23]. ARPES studies performed at $T = 35$ K include scans along M–Γ–M with π and σ polarizations as well as along X–Γ–X with π, σ, circular plus and circular minus polarizations (figures 3(a)–(l)). Solid lines representing dispersions from KKR-CPA calculations (figure 2(e)) are drawn on the experimental data in figures 3(a)–(l). They should be treated as guides to the eye as they are the results of fitting to the intensity map of KKR-CPA calculations. In order to trace the dispersions in the vicinity of μ the spectra were divided by the Fermi–Dirac distribution and are shown in figures 3(m) and (n) with binding energies determined
from fitting energy distribution curves (EDCs) or momentum distribution curves (MDCs) with the Lorentzian function. The experimental and theoretical dispersions are compared in figure 3(o).

A comparison of the band dispersions measured along the Γ–M (figures 3(a), (b), (g), (h)) and Γ–X (figures 3(c)–(f), (i)–(j)) shows that they are quite similar at the Γ point. For π-polarization, a barely visible inner hole-like band (α) (figure 3(m)) can be traced in both directions. The same polarization also yields a very flat quasiparticle band with strong intensity near the Γ point (β1). In fact, due to its high effective mass the dispersion was not measurable and the band exhibits practically constant binding energy determined to be 3–5 meV above the Fermi level. The negligibility of the dispersion was confirmed by the EDCs shown in figure 3(p), which have approximately the same shape at Γ and at ±0.05 Å−1. EDCs from ±0.1 Å−1 at the edges of β1 seem to be more coherent. Their coherent part has the same binding energy but exhibits lower intensity. A contribution from another structure at higher binding energy is also observed. This structure may be evidence of a broadening of the quasiparticle band, incoherent spectral intensity or another hole band. Integrating the EDCs in the range ±0.1 Å−1 over the wavevector yields a peak with a width of 30 meV as shown in figure 3(p). This narrow width, which is also characteristic of single EDCs confirms the quasiparticle nature of this spectral intensity. Raising the temperature to 70 K did not deliver any evidence of electron-like dispersion (not shown).

On the other hand, the spectra obtained with σ-polarization (figures 3(b), (d), (h), (j)) show a dispersion (β2), which looks like the outer hole pocket. It is clear that α corresponds to the inner hole-like band in the calculations. However, the interpretation of β1 and β2 leaves a certain ambiguity. The favoured scenario assumes that these features originate from the same band. This is supported by the circular polarization studies, which yield a continuous dispersion of β1 and β2. Moreover, such an interpretation is in agreement with the band structure calculations (figure 3(o)) as β1 and β2 match well with the calculated middle hole band. However, it has to be remarked that the experimental dispersion exhibits a more ‘kink-like’ shape with mass renormalization near µ when compared to the theoretical one. It is noteworthy that this band changes its orbital character rather abruptly around the Γ point, as β1 and β2 are sensitive to different polarizations in the experiment. One may still consider the other interpretation. The hypothesis that α, β1 and β2 originate from three hole pockets may also be compatible with our data. It may be supported by a possible similarity between S doped and Se doped Fe1+yTe. The band structure at Γ found in FeTe1−ySey before [25–27] consists of three hole-like bands. In the case of FeTe0.55Se0.45 [27] one of the bands also forms a flat dispersion near µ with a narrow quasiparticle peak. An extension of this band is visible as a hole pocket. However, in our case, the hypothesis that β1 originates from the third hole pocket is not indicated directly by the data. Importantly and independently of the interpretation, β1 remains flat and lies close to the chemical potential on a circle with a radius of approximately 0.15 Å−1. Such a situation should result in a spike in the density of states close to µ called a Van Hove singularity (VHs). It is known as an important factor for induction or enhancement of superconductivity. It has already been suggested that VHs may play an important or even more universal role in the formation of superconductivity [42] for a number of compounds.

Let us compare the spectra obtained for superconducting Fe1.03Te0.94S0.06 near the Γ point with the literature results for undoped Fe1+xTe [21–23]. The bands found with σ-polarization by Xia et al [21] are in relative agreement with our spectra. However, for π-polarization, the spectrum of Fe1+xTe consists of a hole pocket with no trace of the flat band at µ. On the other hand, the ARPES studies of undoped Fe1.06Te [22] and Fe1.02Te [23] are characterized by broadened spectra with less clear band topography, which may be similar to [22] or rather different [23] from Fe1.03Te0.94S0.06 results.

It is known that bands in Fe1+yTe1−xSe appear to be strongly renormalized [24–26] when compared to ab initio calculations. In the case of Fe1.03Te0.94S0.06 the inner hole pockets from KKR-CPA calculations fit the experimental spectra quite reasonably (figure 3(o)) and do not indicate strong mass renormalization. However, if the hypothesis of three hole pockets in the experiment was assumed, the agreement between the data and the calculations would be poorer. It is noteworthy that KKR-CPA calculations made for disordered Fe1+yTe0.9S0.1 and LAPW + LO calculations performed for stoichiometric FeTe reveal different effective masses at µ (figure 3(o)). This result shows that the estimation of band renormalization can be uncertain, as it depends on the used approach in band structure calculations. The KKR-CPA approach yields higher effective mass in the theoretical dispersions, what implies lower mass renormalization.

3.3. Photon energy dependent studies

The next important point is band dimensionality, which can be explored by a photon energy dependent study. Therefore, the region of Γ was investigated with energies between 22.5 and 50 eV (figure 4). The outer part of the hole pocket (β2) can always be detected with σ-polarization. The flat dispersion near Γ (β1) can be seen for photon energies of 40, 45 and 50 eV. On the other hand, its intensity is suppressed for 22.5 and 30 eV. There are two optional explanations for this fact: a dispersion along the wavevector component perpendicular to the surface (kz) or a photoionization cross-section effect. To estimate the change of kz for the considered photon energy range one may use the free electron final state (FEFS) model [43] with a typical value of V0 = 15 eV for the inner potential estimated in the case of iron pnictides [44, 45]. If the photon energy is increased from 22.5 to 50 eV the corresponding shift in kz would be 1.06 Å−1, which is approximately equal to the lattice constant in the reciprocal space c∗ = 1.02 Å−1. An assumption of different V0 values between 10 and 25 eV does not change the corresponding shift in kz considerably. Therefore, if the FEFS model is applicable, the spectra for 22.5 and 50 eV should refer to
Figure 4. Incident photon energy dependence of ARPES spectra recorded for Fe$_{1.03}$Te$_{0.94}$S$_{0.6}$ at $T = 35$ K along X–Γ–X in the centre of the Brillouin zone with the following photon energies $h\nu$ and polarizations: (a) 22.5 eV, $\pi$, (b) 22.5 eV, $\sigma$, (c) 30 eV, $\pi$, (d) 30 eV, $\sigma$, (e) 40 eV, $\pi$, (f) 40 eV, $\sigma$, (g) 45 eV, $\pi$, (h) 45 eV, $\sigma$, (i) 50 eV, $\pi$, (j) 50 eV, $\sigma$.

3.4. Analysis of the orbital characters

A photoelectron spectroscopy experiment realized in $\sigma$ or $\pi$ geometry is able to determine the orbital wavefunction parity with respect to the mirror plane, which is defined by the positions of the radiation source, sample and detector (figure 5) [46–48, 21]. Thus, possible orbital characters can...

equivalent regions in the reciprocal lattice. In such a case different matrix elements could be the only explanation for the vanishing spectral intensity ($\beta_1$) for lower photon energies. If the flat band is present for all $k_z$ values, it can be estimated that it covers about 3% of the Brillouin zone volume. Finally, eventual dispersion of $\beta_2$ as a function of $k_z$ was not found, so this band can be considered as two-dimensional.
Figure 5. Schematic presentation of the ARPES experiment with $\pi$-polarized photons (electric field vector in the mirror plane) and $\sigma$-polarized photons (electric field vector perpendicular to the mirror plane). For the sketched configuration $\sigma$ polarized photons detect $d_{xy}$ and $d_{yz}$ orbitals whereas $\pi$-polarized radiation probes $d_{z^2}$, $d_{x^2-y^2}$ and $d_{xz}$ orbitals.

Figure 6. Band structure of stoichiometric FeTe. Contributions of (a) $d_{x^2-y^2}$, (b) $d_{xy}$, (c) $d_{z^2}$ and (d) $d_{xz}/d_{yz}$ orbital characters are represented by band widths (thick bands).

be associated with the observed bands shown in figure 3. In the first considered geometry, the mirror plane is defined by the $z$ axis perpendicular to the sample surface and the $x$ axis corresponding to the $\Gamma$–$M$ direction. The analyser slit is oriented along this plane. The orientation of the Fe-d orbitals dominating the vicinity of the Fermi energy is similar to the case of the iron pnictides [49] with the $x$ and $y$ axes pointing along the corresponding $\Gamma$–$M$ directions. $\pi$-polarized photons excite the states that are even with respect to the considered plane. Consequently, the $d_{xz}$, $d_{x^2-y^2}$ and $d_{z^2}$ orbitals are allowed for the band $\alpha$ along $\Gamma$–$M$ (figures 3(a), (g)). $\beta_1$ will be discussed separately as a special case related to the $\Gamma$ point, which was scanned four times with different geometries and polarizations. $\sigma$-polarized radiation probes states with $d_{xz}$ and $d_{xy}$ orbital character, as they are odd with respect to the mirror plane (figure 5). Hence, $\beta_2$ along $\Gamma$–$M$ (figures 3(b), (h)) may be dominated by these orbital characters. A rotation of the sample such that the mirror plane is along the $\Gamma$–$X$ direction changes the orbital parity related to the plane. Along this direction the orbitals $d_{xz}$ and $d_{yz}$ equally contribute to bands as $d_{xz} + d_{yz}$ or $d_{xz} - d_{yz}$. In this geometry measurements with $\pi$-polarization (figures 3(c), (i)) probing the bands with even symmetry indicate that $\alpha$ can be dominated by $d_{xz} + d_{yz}$, $d_{z^2}$ and $d_{xy}$. On the other hand, the experiment with $\sigma$-polarization (figures 3(d), (j)) reveals that $\beta_2$ should originate from $d_{x^2-y^2}$ and $d_{xy}$ along $\Gamma$–$X$.

Finally, let us consider the $\beta_1$ spectrum. Bands scanned along $\Gamma$–$M$ with $\pi$-polarization (figures 3(a), (g)) can be composed of $d_{xz}$, $d_{x^2-y^2}$ and $d_{z^2}$. However, the same $\Gamma$ point is also scanned along $\Gamma$–$X$ with $\sigma$-polarization (figures 3(d), (j)). The latter measurement yields no intensity at $\Gamma$, which indicates that $d_{x^2-y^2}$ and $d_{xy}$–$d_{xz}$ band characters are not present there. Hence, only the $d_{z^2}$ remains as a dominant character for $\beta_1$. Similar reasoning for the $\Gamma$ point may be done using the spectra obtained with $\pi$-polarization along $\Gamma$–$X$ (figures 3(c), (i)) permitting $d_{xz} + d_{yz}$, $d_{z^2}$ and $d_{xy}$ characters together with the other scan with $\sigma$-polarization along $\Gamma$–$M$ (figures 3(b), (h)) revealing the lack of intensity at $\Gamma$. The last one indicates that $d_{xz}$ and $d_{xy}$ are not present at $\Gamma$, which leads to the same conclusion that mainly $d_{z^2}$ character contributes to the $\beta_1$ spectrum.

The contribution of s-, p- and d-valence orbital characters was also estimated theoretically by means of the LAPW + LO method implemented in the Wien2k package [39] (figure 6). The calculations were realized for stoichiometric FeTe. The results confirm that d-orbitals dominate the band structure in
the vicinity of the Fermi energy (other orbital projections are not shown in figure 6). The hole bands $\alpha$ and $\beta_2$ appearing around the $\Gamma$ point have their counterparts in the theoretical results. Although it is not obvious to what extent the calculations for pure FeTe are reliable for Fe$_{1.05}$Te$_{0.94}$S$_{0.06}$, they can narrow down the list of possible band characters. The calculations yield that the $\alpha$ band has mainly $d_{xz}/d_{yz}$ orbital character, while $\beta_2$ is dominated by $d_{yz}/d_{xy}$ with some contribution from $d_{z^2}$ along $\Gamma$–X. This is in agreement with the experimental results obtained both along $\Gamma$–M and $\Gamma$–X directions. In contrast, the calculations for FeTe do not reveal the flat band at the Fermi energy with dominant $d_{z^2}$ orbital character, which would correspond to $\beta_2$. In this aspect they are not compatible with the experiment for Fe$_{1.05}$Te$_{0.94}$S$_{0.06}$. One may expect that S doping in the Fe$_{1+x}$Te$_{1-y}$S$_y$ system may have a particular effect on the $d_{z^2}$ orbital as it results in shrinking the $c$ lattice constant.

4. Conclusions

The band structure of superconducting Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$ was studied along the $\Gamma$–X and $\Gamma$–M directions by ARPES. An increased spectral intensity at $\mu$ is observed near the $\Gamma$ and M points. In particular, two hole bands ($\alpha$ and $\beta_2$) are found around $\Gamma$ with a high intensity quasiparticle peak ($\beta_1$) located close to $\mu$, with no evidence of dispersion. This latter feature has mainly $d_{z^2}$ orbital character and is interpreted as the maximum of the $\beta_2$ hole band or as evidence of another hole pocket. Such a band structure yields a high degree of states at the chemical potential, interpreted as a Van Hove singularity. Measurements performed with variable photon energy show no dispersion of the $\beta_2$ hole band as a function of $k_z$. Hence, it is considered to be two-dimensional. The flat part of the band located at $\mu$ has a reduced intensity for the photon energies of 30 and 22.5 eV, which is attributed to a low photoionization cross-section. The band structure obtained from KKR-CPA calculations includes the broadening due to disorder and exhibits three hole pockets in $\Gamma$ and two electron pockets at M. Further LAPW-LO calculations performed for stoichiometric FeTe lead to a band topography, which is in reasonable agreement with the KKR-CPA results and the experiment for Fe$_{1.03}$Te$_{0.94}$S$_{0.06}$. The orbital characters calculated with the LAPW-LO method agree with the experimental results for $\alpha$ and $\beta_2$ dispersions but are inconsistent with the $d_{z^2}$ character observed for the flat $\beta_1$ spectrum.

Acknowledgments

HS, FF and FR acknowledge the support by the DFG through FOR1162. The study has been supported by Polish National Science Centre grant 2011/01/B/ST3/00425. PZ acknowledges use of the equipment at the UMD Nanoscale Imaging Spectroscopy and Properties Laboratory. The research leading to these results has received funding from the European Community’s Seventh Framework Programme (FP7/2007-2013) under grant agreement number 226716.

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