Three Dirac points on the (110) surface of the topological insulator Bi$_{1-x}$Sb$_x$

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Abstract. Topological insulator surfaces support metallic surface states with closed Fermi contours, encircling an odd number of Dirac points. Experimental studies have so far concentrated on surfaces with only one Dirac point, but three Dirac points can be expected for certain surface orientations of several topological insulator materials. Here we experimentally realize the Bi$_{1-x}$Sb$_x$(110) surface for which an electronic structure with three Dirac points has been predicted (Teo et al 2008 Phys. Rev. B 78 045426), in contrast to the closed-packed (111) surface of the same material that supports only one Dirac point. We study the electronic structure of Bi$_{1-x}$Sb$_x$(110) with angle-resolved photoemission and tight-binding calculations. We observe several metallic surface states, confirming not only the expectation that a topological insulator should be enclosed by metallic surfaces on all faces, but also the prediction of the surface state topology. Tight-binding calculations of the electronic structure are found to reproduce the expected topology of the surface states but they show
one Dirac point that is not observed in the experiment, in the mirror line of the surface Brillouin zone. As in the case of Bi$_{1-x}$Sb$_x$(111), this can be ascribed to an incorrect value of the mirror Chern number in the tight-binding parameters employed for the calculation. The quantitative agreement of the tight-binding calculation and the experiment is poorer than in the case of the (111) surface, something that is ascribed to the existence of dangling bonds on the (110) surface.

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1. Introduction

Three-dimensional topological insulator (TI) crystals consist of an insulating bulk enclosed by metallic surfaces, and detailed theoretical predictions about the surface state band topology and spin texture are available [1–7]. While several TI materials are currently known, the existence and topology of the metallic surface states have rarely been probed for different surfaces orientation of a given material [8]. For most TIs, such as Bi$_{1-x}$Sb$_x$ and Bi$_2$Se$_3$, the most studied surface is the closed-packed (111) surface that can be obtained by cleaving the bulk crystal.

Being able to change the surface orientation of a TI under investigation would provide more subtle information than the mere confirmation of a bulk crystal enclosed by metallic surfaces, and specific predictions about the orientation and termination-dependent electronic structure could be verified. For instance, the predicted Fermi contour for many TI surfaces consists of an odd number of Dirac cones around the Brillouin zone centre $\bar{\Gamma}$ (see e.g. [9–13]) but more complex scenarios with Dirac cones around three time-reversal invariant momenta (TRIMs) in the surface Brillouin zone have been predicted for non-(111) surfaces of Bi$_{1-x}$Sb$_x$ ($x > 0.09$) [1] and for SmB$_6$(001) [14]. In fact, the possibility of finding three Dirac points depends on the bulk band topology: if the bulk parity inversion only takes place at the Brillouin zone centre $\Gamma$, this leads to an odd number of closed Fermi contours around the surface Brillouin zone centre $\bar{\Gamma}$ for every possible surface orientation [8], even though it might be possible to change this by the surface termination [1], as discussed in more detail below. However, if the bulk parity inversion happens at another bulk TRIM, one should be able to change the surface state topology by choosing different surface orientations. TIs with a parity inversion not (only) at $\Gamma$ are Bi$_{1-x}$Sb$_x$ (parity inversion at every bulk TRIM except $L$ [1]), PbBi$_2$Te$_4$ (parity inversion at $Z$ [12]) and SmB$_6$ (parity inversion at $X$ [14]).

While the surface topology for any desired surface orientation can be readily predicted once the bulk electronic structure of a TI with inversion symmetry is known [2], the experimental
preparation of any surface orientation is not easy. Feasible methods for preparing TI surfaces are cleaving \[9, 10\], a combination of cutting, polishing and \textit{in situ} cleaning, as well as epitaxial growth \[15–17\]. While cleaving has so far been used to prepare the very stable (111) surfaces of Bi\(_{1-x}\)Sb\(_x\) and the Bi\(_2\)Se\(_3\)/Bi\(_2\)Te\(_3\) family, the same surfaces can also be obtained by epitaxial growth \[15, 18\], as well as Bi\(_2\)Se\(_3\)(221)\[8\] and HgTe(001) \[17\]. Cutting and \textit{in situ} cleaning could in principle give any desired surface direction, but the approach is hindered by the small size of most crystals, their anisotropy and the high likelihood to off-set the delicate stoichiometry near the surface during the \textit{in situ} cleaning process.

Here we experimentally realize Bi\(_{1-x}\)Sb\(_x\)(110), a surface of a TI that cannot be prepared by cleaving a bulk crystal, and we probe the surface state topology by angle-resolved photoemission (ARPES). As expected, this surface also supports metallic states but the change in surface orientation drastically modifies the band topology, leading to three Dirac points instead of one, as found for the (111) surface \[9\]. In this way, a valley degree of freedom is added to a TI surface, much like in graphene but without the additional spin degree of freedom.

After this brief introduction, we address the general issue of the surface state topology and compare the case of Bi\(_{1-x}\)Sb\(_x\)(110) to that of the prototypical TI Bi\(_2\)Se\(_3\) which does not allow the creation of surfaces with three Dirac cones. In the following sections, we describe the experimental and computational details of our study and give the experimental results for the electronic structure of Bi\(_{1-x}\)Sb\(_x\)(110) compared to Bi(110). Subsequently, we discuss the results of a tight-binding calculation for Bi\(_{1-x}\)Sb\(_x\)(110). We end the paper with some conclusions.

2. Surface state topology

Before discussing the experimental results, we briefly review the theoretical predictions for the surface state electronic structure of the TIs, following the treatment by Teo \textit{et al} \[1\]. The existence and topology of a surface Fermi contour is derived from the parity invariants \(\delta(\Gamma_i)\) for the eight bulk TRIMs \(\Gamma_i\) in the Brillouin zone. \(\delta(\Gamma_i)\) can take the values of +1 and \(-1\), signalling a conventional parity and a parity inversion, respectively. Based on these values, the surface fermion parity \(\pi(\Lambda_a)\) for the four surface TRIMs \(\Lambda_a\) can be evaluated by

\[
\pi(\Lambda_a) = (-1)^n_b \delta(\Gamma_i) \delta(\Gamma_j),
\]

where \(n_b\) is the number of occupied, spin-degenerate bulk bands \[1\]. \(\pi(\Lambda_a)\) can then be used to predict the number of (non-spin-degenerate) closed Fermi contours around a surface TRIM. For \(\Lambda_a = 1\), none or an even number of enclosing contours is expected; for \(\Lambda_a = -1\) an odd number of enclosing contours will result.

Note that frequently, instead of stating that there is a closed Fermi contour around a TRIM, one finds the statement that there is a Dirac point at this TRIM and we also use this expression in the present paper when we speak of one or several Dirac points in the surface Brillouin zone. Note, however, that these concepts are not exactly the same. The theory does not actually predict the existence of Dirac points because these can lie within the projected bulk bands at the actual TRIMs (either in the valence band or in the conduction band). The theory merely predicts the existence of closed Fermi contours. When we speak of a certain number of Dirac points per surface Brillouin zone, we therefore mean the topologically required surface state band crossings around a TRIM. There can be other crossings as well, caused by coincidence or crystal symmetries but we do not count these here.
Figure 1 now illustrates these predictions for the (111) and (110) surfaces of Bi$_2$Se$_3$ and Bi$_{1-x}$Sb$_x$. For Bi$_2$Se$_3$(111) (figure 1(a)) the application of (1) is particularly simple: the bulk parity inversion happens only at the bulk $\Gamma$ point, so $\delta(\Gamma) = -1$ while $\delta = 1$ for the other bulk TRIMs. Moreover, $n_b$ in (1) is even ($n_b = 14$), so that the bulk parity inversion causes a negative surface fermion parity on the $\Gamma$ surface TRIM but not on $M$. Interestingly, the topological prediction for Bi$_{1-x}$Sb$_x$(111) (in the topologically non-trivial phase with $x > 0.09$) is exactly the same but for entirely different reasons. In the bulk, a parity inversion takes place at every TRIM except $L$. Projecting this out, one would obtain the opposite situation as for Bi$_2$Se$_3$(111), namely a negative surface fermion parity on $M$ and a positive at $\Gamma$, were it not for the fact that the number of bulk bands is odd ($n_b = 5$) in Bi$_{1-x}$Sb$_x$, so that (1) gives the same result for Bi$_{1-x}$Sb$_x$(111) as for Bi$_2$Se$_3$(111). In the topologically trivial phase ($x < 0.09$), there is a bulk parity inversion at every TRIM, leading to a negative surface fermion parity for both $\Gamma$ and $M$.

The fact that the surface state topology for Bi$_2$Se$_3$ and Bi$_{1-x}$Sb$_x$ is identical for the (111) surface is therefore, in a way, a mere coincidence. For other surface orientations, this is not necessarily so. In fact, it is easy to see that the topology for different Bi$_2$Se$_3$ surface orientations is always the same: the bulk parity inversion at $\Gamma$ will always project out to the surface $\Gamma$ point and thus the surface electronic structure will always be expected to consist of an odd number of Fermi contours around $\Gamma$ and none around the other surface TRIMs. A surface electronic structure consistent with this prediction has recently been reported for Bi$_2$Se$_3$(221) [8]. It consists of an elongated electron pocket around the $\Gamma$ point. Note, however, that one way to change the entire surface state topology may be to choose a termination in a different position of the quintuple layer, i.e. at different locations with respect to the bulk inversion centres [1]. Such a change could then lead to a closed Fermi contour around every surface TRIM except $\Gamma$.

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In contrast to Bi$_2$Se$_3$, other surface orientations of Bi$_{1-x}$Sb$_x$ can be expected to have an entirely different topology than an odd number of closed contours around $\bar{\Gamma}$ because the only bulk TRIM without parity inversion ($L$) is projected out onto different surface TRIMs. Moreover, it is the bulk parity value $\delta$ that changes at $L$ when going from the topologically trivial situation for $x < 0.09$ to the TI at $x > 0.09$. The situation for Bi$_{1-x}$Sb$_x$(110) is shown in figure 1(b). The bulk $L$ point now projects out to the $\bar{X}_2$ surface TRIM, such that we obtain a negative surface fermion parity for every surface TRIM except $\bar{X}_2$. Thus, the number of surface Dirac points changes from one to three.

Changing the bulk topology of Bi$_{1-x}$Sb$_x$ to the trivial phase for $x < 0.09$ would then switch the surface fermion parity from 1 to $-1$ at $\bar{X}_2$ and therefore require this point to be surrounded by a closed Fermi contour as well. This would then correspond to an even number of Dirac points (four) in the surface Brillouin zone. Note, however, that for $x < 0.07$ the material also ceases to be an insulator and becomes a semimetal instead. Therefore, the topological predictions do not have to be strictly valid any more.

3. Experimental and theoretical methods

We grow epitaxial films of the TI Bi$_{1-x}$Sb$_x$ in the (110) orientation by simultaneous evaporation of Bi and Sb onto a Bi(110) surface. The latter had previously been cleaned by cycles of Ne ion sputtering and annealing. Since $x$ is quite small in the TI phase (0.09 < $x$ < 0.18), the lattice mismatch between the Bi substrate and the film is so small [19] that the growth is quasi-homoepitaxial, resulting in a high-quality Bi$_{1-x}$Sb$_x$(110) film. While growing the film, the substrate was held at a temperature of 403 K. Data were taken for different film thicknesses and compositions. The data shown in this paper were obtained from a film with a thickness of approximately 25 double layers and $x \approx 0.14$ (here the term double layer is used to group the first and second layer of the A7(110) surface. These are almost at the same height [20–22]). ARPES data from clean Bi(110) are also shown for comparison. The growth rate and chemical composition of the film were determined by inspecting the shallow Sb 4d and Bi 5d core levels, as in [16]. The order of the films was confirmed by the observation of sharp reflections in a low-energy electron diffraction pattern and by the existence of sharp features in the observed band structure.

ARPES data were taken at the SGM-3 beamline of the synchrotron radiation source ASTRID [23]. The energy and angular resolution for ARPES measurements were better than 20 meV and 0.2°, respectively. Data were collected with photon energies between 14 and 32 eV in order to support the interpretation of states as surface states by the fact that their dispersion does not depend on the photon energy. The sample temperature during the measurements was 80 K.

The bulk Fermi surface projections and band structure surface projection were calculated using the tight-binding parameters of Liu and Allen [24]. For the alloy, the parameters were interpolated following the method in [1]. For the surface state band structure calculation in the last section of the paper, a sp$^3$ Slater–Koster [25] tight-binding model was used, which includes third-neighbour hopping parameters and spin–orbit coupling. Based on this, the surface states dispersion was calculated using a transfer-matrix technique and a Green’s function approach [26, 27]. The Green’s function of the semi-infinite surface was generated from the transfer matrix which was calculated self-consistently. Its imaginary part represents the surface state dispersion as observed in ARPES experiments.
Figure 2. (a), (d) Core level spectra in the Sb 4d and Bi 5d region for Bi(110) and a 25 bilayer film of Bi$_{0.86}$Sb$_{0.14}$(110) grown epitaxially on Bi(110) (taken with a photon energy of $h\nu = 80$ eV). (b), (e) Photoemission at the Fermi level for the two samples ($h\nu = 18$ eV, dark corresponds to high intensity). The exact position of the high symmetry points is indicated by purple dots. (c), (f) Surface Brillouin zone with topological predictions for the two cases. Blue circles denote the topologically predicted closed Fermi contours (an odd number of such contours). The yellow contours are experimentally found Fermi contours with no topological relevance. The red areas correspond to the projected bulk Fermi surface for Bi(110).

4. Angle-resolved photoemission results

Figures 2(a) and (d) show the core level spectra in the Sb 4d and Bi 5d regions for clean Bi(110) and a Bi$_{0.86}$Sb$_{0.14}$(110) film, respectively. From such spectra, we can deduce the chemical composition of the film, assuming a random distribution of Sb in the alloy. Our determination of the film composition is consistent with that of [16].

The $k$-resolved photoemission intensity at the Fermi level for the two samples is shown in figures 2(b) and (e). Several surface-related Fermi contours can be identified. For Bi(110) the result is very similar to earlier studies of this surface [28–30] but the improved spectrometer resolution in the present work reveals some previously unobserved details. In particular, it is clearly seen that the $\bar{X}_1$ TRIM is surrounded by a small closed Fermi contour that will be shown to be an electron pocket. The other observed features have been reported before. They consist of two closed contours around $\bar{\Gamma}$ and $\bar{M}$ (both hole pockets), as well as a shallow electron pocket.
on the $\bar{M} - X_1$ line. Furthermore, a faint and broad feature of higher photoemission intensity can be seen near the $X_2$ point. This has been previously interpreted as bulk-related [28].

The topological predictions for Bi(110) are given in figure 2(c). As explained in the previous section, one expects every surface TRIM to be encircled by one closed Fermi contour (or by a higher odd number); and this is schematically outlined by blue filled circles around the TRIMs. The experimental results do confirm the expected structures around $\Gamma$, $X_1$, and $M$ but apparently not around $X_2$. However, as Bi is a semimetal, this does not contradict the theoretical predictions that are supposed to hold strictly only for insulators. In fact, the topologically required band crossings can take place inside the projected bulk Fermi surface (red area in the figure 2(c)). The yellow structures in figures 2(c) and (f) are Fermi contours that are observed experimentally but that have no topological significance, something that can already be seen by the fact that they are not encircling any TRIM. They are given only to permit an easier comparison between prediction and experimental result.

Figures 2(e) and (f) give the corresponding plots for Bi$_{0.86}$Sb$_{0.14}$(110). Figure 2(e) is, at first glance, very similar to the result for Bi(110). The contours around $\bar{M}$ and $X_1$ as well as the electron pocket on the $\bar{M} - X_1$ line appear slightly bigger than for Bi(110) and start to merge into each other. The quantum phase transition from topologically trivial Bi to non-trivial Bi$_{1-x}$Sb$_x$ should be reflected in a change of the surface state dispersion around the $X_2$ point. In particular, there should not be any closed surface Fermi contour around $X_2$ for the TI. Such a contour is indeed absent from the data but it is not clearly observed for Bi(110) either. In both cases, a streak of high photoemission intensity in the $\bar{\Gamma} - X_2$ direction is seen.

In figure 3 the situation near $X_2$ is further explored by high-resolution scans along $\bar{\Gamma} - X_2$ for both Bi(110) and Bi$_{0.86}$Sb$_{0.14}$(110). In figures 3(a) and (c) scans taken at $h\nu = 18$ eV are plotted together with the projected band structure. In figures 3(b) and (d) data for a range of photon energies are shown. An inspection of the entire data set reveals that the surface state dispersion in this direction is quite different in the two cases: both surfaces share the hole pocket around $\bar{\Gamma}$, but whereas the band forming this pocket disappears into the projected band states for Bi$_{0.86}$Sb$_{0.14}$(110), its dispersion reaches a binding energy maximum for Bi(110) before it disperses back towards the Fermi level. It merges with the projected bulk bands in the immediate vicinity of the $X_2$ point. There, the intensity from the band is lost. While the topological prediction are only of limited meaning for a semimetal, we can speculate that this band could indeed lead to a small closed Fermi surface feature around $X_2$ (a hole pocket). With the state disappearing in the bulk continuum, this appears to be of limited significance but the comparison with Bi$_{0.86}$Sb$_{0.14}$(110) clearly shows that the quantum phase transition to the TI phase proceeds by removing the Fermi contour around $X_2$ that would be created by this band in the absence of bulk states.

Both surfaces show some photoemission intensity at the Fermi level close to $X_2$. For Bi(110), this can clearly be due to the projected bulk bands and it has previously been interpreted in this way [28]. For Bi$_{0.86}$Sb$_{0.14}$(110) the origin of this intensity is not clear. While the feature appears quite broad and is therefore likely to be of bulk origin, there should not be any bulk states in the projected bulk band gap of the film. In order to explore this further, consider the photon energy scans taken around $X_2$ for Bi(110) and Bi$_{0.86}$Sb$_{0.14}$(110) in figures 3(b) and (d), respectively. Changing the photon energy strongly affects the photoemission intensity distribution near $X_2$. We can clearly distinguish two broad structures on either side of $X_2$. For photon energies below $h\nu = 18$ eV the feature in the first...
Figure 3. Detailed electronic structure along the $\Gamma - \bar{X}_2$ line for (a) Bi(110) and (c) Bi$_{0.86}$Sb$_{0.14}$(110) ($h\nu = 18$ eV). Dispersing surface states are marked by dashed blue lines as a guide to the eye. The shaded areas dots denote the projected bulk band structure (conduction band blue and valence band red). The inset shows the surface Brillouin zone with the topological predictions in blue, additional experimentally found Fermi contours in yellow and projected bulk Fermi surfaces in red. The magenta lines in the inset mark the scan direction. (b), (d) Photon energy-dependent data near $\bar{X}_2$ for Bi$_{0.86}$Sb$_{0.14}$(110) in order to elucidate the nature of the in-gap photoemission intensity near that point. $\bar{\Gamma}$ is the centre of the (first) surface Brillouin zone corresponding to the normal emission direction and $\bar{\Gamma}'$ is the centre of the neighbouring Brillouin zone.

Brillouin zone (towards $\bar{\Gamma}$) is most intense; for $h\nu > 18$ eV the feature in the neighbouring zone (towards $\bar{\Gamma}'$) is most intense; and at $h\nu = 18$ eV the intensity is approximately symmetric.

While no clear sign of dispersion in either $k_\parallel$ or $k_\perp$ is observed, the two features are most likely of bulk origin. An inspection of the projected bulk band structure in figure 3(b) shows that bulk states at the Fermi energy on either side of $\bar{X}_2$ would be expected for a very small $n$-doping of the film. Such bulk states would be expected to have a dispersion with $k_\perp$ but if the binding energy maximum reached in this dispersion is barely below the Fermi energy, one would not expect to actually observe the dispersion. Instead, one would merely expect the state to be clearly observable for a photon energy that leads to emission from the state at the highest binding energy and not observable otherwise. This behaviour is consistent with figure 3(d). Moreover, the observed intensity changes are very similar to those for the conduction band minimum of the clean Bi(110) surface shown in figure 3(b). It is also apparent that a downward shift of the entire projected band structure in figure 3(c) would lead to a better qualitative agreement with the diffuse, and presumably bulk-related photoemission intensity. Finally, the projection of the bulk conduction band minimum is not only found near $\bar{X}_2$ but also at $\bar{X}_1$. Therefore, one would
Figure 4. Detailed electronic structure around the $\bar{X}_1$ point of $\text{Bi}_{0.86}\text{Sb}_{0.14}(110)$, showing the detailed dispersion and character of the states that give rise to a closed Fermi contour around this point. Panels (a) and (b) show scans around $\bar{X}_1$ towards $\bar{\Gamma}$ and $\bar{M}$, respectively. The directions are also marked by the magenta dashed lines in the insets. The projected bulk band structure is outlined by the shaded areas. The second inset in (b) shows a magnification of the situation very close to $\bar{X}_1$ with the colour scale chosen such that the intensity from the shallow electron pocket is saturated. This clearly reveals the Dirac-like crossing of the bands at $\bar{X}_1$.

also expect to observe some photoemission intensity at the Fermi energy near that point. This is indeed found and we shall discuss it below in connection with figure 4. Upon close inspection, some photoemission intensity within the closed surface state Fermi contour encircling $\bar{X}_1$ can already be discerned in figure 2(e). The important conclusion from these considerations is that the topological predictions for $\text{Bi}_{0.86}\text{Sb}_{0.14}(110)$ appear to be strictly fulfilled near $\bar{X}_2$: while we do observe some, most likely bulk-related, photoemission intensity near $\bar{X}_2$, we can rule out that a surface state Fermi contour encircles $\bar{X}_2$.

The observation of the conduction band minimum near $\bar{X}_1$ and $\bar{X}_2$ suggests that the $\text{Bi}_{0.86}\text{Sb}_{0.14}(110)$ film is slightly $n$-doped. Such doping could be caused by the interplay of surface and bulk electronic structure of the film. If we assume that the density of interface states between the Bi(110) substrate and the $\text{Bi}_{0.86}\text{Sb}_{0.14}(110)$ is very small, the surface electronic structure of the film could be alone responsible for the bulk doping. When estimating the size of the four Fermi contours (hole pockets around $\bar{\Gamma}$ and $\bar{M}$, electron pockets around $\bar{X}_1$ and between $\bar{X}_1$ and $\bar{M}$), we find an electron density of $\approx 2.5 \times 10^{13}$ cm$^{-2}$ and a hole density of $\approx 3.8 \times 10^{13}$ cm$^{-2}$. The total surface charge is therefore dominated by holes and this has to be compensated by an $n$-doping of the bulk film.

A final topological prediction for $\text{Bi}_{0.86}\text{Sb}_{0.14}(110)$ is the existence of a closed Fermi contour around $\bar{X}_1$. This contour can already be seen in figures 2(e), and figure 4 gives a more detailed view of the band structure around this TRIM along $\bar{X}_1$-$\bar{\Gamma}$ and $\bar{X}_1$-$\bar{M}$. The scans reveal that the closed Fermi contour around $\bar{X}_1$ is an electron pocket. In fact, the band giving rise to it merges with the lower Rashba-split surface state bands originating from $\bar{\Gamma}$ and $\bar{M}$ to form a
Dirac point at $\bar{X}_1$ but this Dirac point is situated within the projected valence band. Nevertheless, the Dirac-like crossing of the states can actually be observed in the $\bar{X}_1 - \bar{M}$ direction when the intensity is scaled such that the other features in the scan are saturated (see inset in figure 4(b)). This situation and the shape of the Fermi contour around $\bar{X}_1$ is similar to that on Sb(110), i.e. the case of $x = 1$ [31].

Note that figure 4(a) shows some photoemission intensity at the Fermi energy near $\bar{X}_1$ that does not derive from the surface states. This is again ascribed to the bulk conduction band minimum that is visible due to a slight $n$-doping of the film, consistent with the results near $\bar{X}_2$ in figure 3. One would expect the same intensity to be seen in figure 4(b), especially since both sub-figures are cuts through the same data set. The reason why there is no clear sign of the bulk-derived intensity in that figure is merely the overall scaling of the intensity. The photoemission intensity from the shallow electron pocket is so strong that weaker features are not visible simultaneously.

5. Tight-binding calculations

We explore the electronic structure for Bi$_{1-x}$Sb$_x$(110) by Green’s function calculations for the semi-infinite bulk, as described in the Methods section. Figure 5(a) shows the resulting Fermi surface for Bi$_{0.86}$Sb$_{0.14}$(110) which is in excellent qualitative agreement with the experimental result: we find one closed Fermi contour around each of the $\bar{\Gamma}$, $\bar{M}$ and $\bar{X}_1$ TRIMs and none around $\bar{X}_2$. The only point of a qualitative disagreement is the presence of a very small Fermi contour feature along $\bar{\Gamma} - \bar{X}_2$ that is not observed in the experiment. The feature is so small that it is hard to discern in figure 4(a) and it is therefore emphasized by a yellow circle.

The situation is further explored by a surface band structure calculation for the lines connecting the surface TRIMs shown in figure 4(b). Here we see that while the topological character of the Fermi contour agrees well between experiment and calculation, the detailed dispersion does not. Most strikingly, the Dirac points at both $\bar{\Gamma}$ and $\bar{M}$ are occupied in the calculation, giving rise to large electron pockets around these points. In the experiment, on
the other hand, the Dirac points are unoccupied such that the Fermi contour features are hole pockets. This is also the case in first principles calculations for Bi(110) [29] and Sb(110) [31]. The failure of the calculation to reproduce the data quantitatively is hardly surprising because the bulk-derived hopping parameters do not account for the strong changes in hybridization and electronic structure at the surface. Even for the closed-packed (111) surface the detailed dispersion obtained in this way [1] does not agree with the experimental one [9], and for the (110) surface the application of bulk-derived hopping parameters to describe the surface band structure is even more questionable because of the presence of dangling bonds on this surface [28]. Knowing the character of the surface Fermi features, we can also state that the situation in figure 5 would correspond to a strongly electron-doped surface since all the Fermi surface features are electron pockets. In the experiment, on the other hand, we have observed an overall hole doping.

It is quite remarkable that the Fermi contour derived from the calculation does agree with the topological predictions. Consider the dispersion in the $\bar{M} - \bar{X}_1$ and $\bar{X}_1 - \bar{\Gamma}$ direction. Two Fermi level crossings are found in each direction, forming the electron pockets around $\bar{X}_1$ and the respective other TRIM. Both Fermi level crossings could be removed by slightly changing the dispersion of the band but this does not happen. The calculation’s topology agrees with the fundamental prediction.

We briefly discuss the origin of the tiny electron pocket in the $\bar{\Gamma} - \bar{X}_2$ direction. It is caused by a crossing of the bands in this direction, as seen in figure 4(b). Its existence is not required by the fundamental topological predictions outlined for this surface above, consistent with the fact that it does not enclose any TRIM. However, it is still topologically protected but, in contrast to the other states, by crystal symmetry and not by time-reversal symmetry. The $\bar{\Gamma} - \bar{X}_2$ direction is also the mirror line on the surface and it has been found for Bi$_{0.86}$Sb$_{0.14}$(111) that using the interpolated tight-binding parameters of Liu and Allen [24] leads to an equivalent additional crossing in the mirror line of that surface ($\bar{\Gamma} - \bar{M}$). Moreover, it has been shown that the additional crossing between the states is enforced by an incorrect mirror Chern number in the tight-binding parameters [1]. An equivalent spurious crossing is therefore expected, and found, for the (110) surface.

6. Conclusion

We have been able to investigate the Fermi contour and surface state dispersion of Bi$_{0.86}$Sb$_{0.14}$(110) by growing the topologically non-trivial phase as a thin epitaxial film on Bi(110). While the overall electronic structure of Bi$_{0.86}$Sb$_{0.14}$(110) and Bi(110) is very similar, the quantum phase transition to a TI is caused by a small change in the surface state dispersion near the $\bar{X}_2$ point. The experimental Fermi contour of Bi$_{0.86}$Sb$_{0.14}$(110) is found to be in excellent agreement with the theoretical predictions for this surface. This is also reproduced by Green’s function calculations using bulk tight-binding parameters. However, while the calculations reproduce the qualitative Fermi contour the detailed dispersion of the states does not agree well with the experimental result.

The Fermi contour of Bi$_{1-x}$Sb$_x$(110) is substantially more complex than for the (111) surface of the same material or the predictions of the non-(111) surfaces of Bi$_2$Se$_3$-type TIs. Indeed, this illustrates the design possibilities when exploiting the surface orientation of a TI. The example shown here is particularly interesting because it leads to the experimental realization of a TI surface with three Dirac points instead of one. Interestingly, this adds a valley
degree of freedom to the topological Dirac fermions, something that is currently attracting great attention in the case of graphene [32, 33] where the additional valley degree of freedom could be used to encode information. Finally, it should be possible to use the same strategy of nearly homo-epitaxial growth for the construction of quasi one-dimensional surface states on three-dimensional TIs, as already found for the vicinal parent surface Bi(114) [34].

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