Evolution of surface states of antiferromagnetic topological insulator MnBi$_2$Te$_4$ with tuning the surface magnetization

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Abstract

The interplay between magnetism and topologically non-trivial electronic states is an important subject in condensed matter physics. Recently, the stoichiometric intrinsic magnetic material MnBi$_2$Te$_4$ provides an ideal platform to study the magnetic topological phenomena, such as quantum anomalous Hall effect, axion insulator state, topological magnetoelectric effect. However, it is still controversial whether the topological surface state in the (111) plane is gapped or not. Here, we develop an effective method to study different surface magnetizations based on first-principles calculations. Then we investigate the band dispersions, the Fermi surfaces (FSs), the quasiparticle interferences (QPIs) and the spin texture of topological surface states of MnBi$_2$Te$_4$ with tuning the surface magnetization. We find that the surface magnetization has significant effects on the surface states. Our results also indicate that the symmetry breaking of FSs and QPIs may be a useful way to determine the possible surface magnetization of MnBi$_2$Te$_4$.

1. Introduction

Topological materials and topological states have become one of the main themes of condensed matter physics [1–4], with the successive discoveries of the quantum spin Hall effect [5, 6], the quantum anomalous Hall (QAH) effect [7, 8], the topological insulator [9–11], the topological semimetal [12, 13] and the topological superconductivity [14]. Recently, the interplay between the magnetism and the topologically nontrivial electronic states attracted great attention in the field. As one of the most important progresses, the QAH effect was firstly predicted and experimentally realized in Cr-doped (Bi, Sb)$_2$Te$_3$ thin films [7, 8], where the dissipationless quantized Hall conductance is obtained without external magnetic field. However, the working temperature is very low (∼30 mK) and its physical picture also seems hard to understand due to the magnetic impurity doping induced disorder.

Recently, the stoichiometric magnetic material MnBi$_2$Te$_4$ was successfully synthesized in experiments [15–17]. It hosts both the intrinsic A-type anti-ferromagnetism (AFM) and topologically nontrivial electronic states [18, 19], so it provides an ideal material platform to study the various intrinsic magnetic topological states, such as, the QAH effect [20, 21], the axion insulator [18, 22, 23], the topological magnetoelectric effect [24–26], and the ideal magnetic Weyl semimetal [18, 19, 27], most of which have been successfully observed in experiments. Because of the A-type AFM with the out-of-plane magnetic anisotropy, the topological state on the (111) surface is predicted to be gapped by first-principles calculations [18, 19, 27]. However, there is still a debate on whether its topological surface states on the (111) surface are gapped [17, 28–30] or gapless [16, 31–33]. Some measurements of angle resolved photoemission spectroscopy (ARPES) show the almost gapless surface states [31–33], which is different from theoretical predictions [18, 19]. By considering that the surface electronic states should be sensitive
with the surface magnetization, possible surface magnetic configurations to the gapless surface states were recently proposed to produce gapless surface states [32]. In this work, we investigate the evolution of topological surface states of MnBi₂Te₄ through tuning the surface magnetization, with first-principles calculations. We find that the surface magnetization has significant effects on the energy gap, Fermi surfaces (FSs) with the spin texture and quasiparticle interferences (QPIs) of surface states. Our results also indicate that the symmetry breaking of FSs and QPIs of surface states may a useful way to determine the possible surface magnetization of MnBi₂Te₄.

The organization of this paper is as follows. In section 2, we show the crystal structure and the bulk electronic structure of MnBi₂Te₄. In section 3, we develop a Wannier-based tight-binding (TB) method to consider the surface magnetization. In section 4, we investigate the evolution of topological surface states through tuning the surface magnetization. Conclusions are summarized in section 5.

2. Crystal structure and bulk electronic structure

MnBi₂Te₄ crystallizes in a rhombohedral crystal structure with the space group $D_{5d}^1$ (no. 166) with seven atoms in one unit cell. As shown in figures 1(a) and (d), the seven atoms (Te–Bi–Te–Mn–Te–Bi--Te) form a septuple layer (SL) along the $z$-direction. It is weak van der Waals coupling between neighboring SLs, and the strong chemical bonding within each SL. Experimental results and theoretical calculations indicate that the magnetic ground state of MnBi₂Te₄ is an A-type AFM with the out-of-plane easy axis. Its magnetic exchange type is ferrimagnetic within each SL in the $xy$ plane and AFM between neighboring SLs [17, 18, 34], as schematically shown in figure 1(a). Due to the AFM order, the unit cell doubles along the $z$-direction. We denote the magnetic ground state as the AFMz state in figure 1(a), while the magnetic order in figure 1(d) is as the AFMx state. Both AFMz and AFMx MnBi₂Te₄ have the inversion symmetry $P$ with the inversion center at the Mn layer. AFMz has the three-fold rotation symmetry $C_{3z}$ along the $z$-axis, but $C_{3z}$ is broken in AFMx MnBi₂Te₄ due to the magnetization along $x$-axis. Though the time reversal symmetry $\Theta$ is broken for both AFMz and AFMx MnBi₂Te₄, a combined time–space symmetry $S = \Theta \tau_{1/2}$ is preserved, where $\tau_{1/2}$ is the half translation connecting nearest opposite spin Mn atoms [18].
Table 1. Matrix element $\langle \sigma, p | L \cdot S | \sigma, p \rangle$ of the SOC term with respect to the spin direction along $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ and $p$-orbitals for the SOC term $H^{soc}$.

| $\uparrow, p_x$ | $\uparrow, p_y$ | $\uparrow, p_z$ | $\downarrow, p_x$ | $\downarrow, p_y$ | $\downarrow, p_z$ |
|----------------|----------------|----------------|----------------|----------------|----------------|
| $\uparrow, p_x$ | 0 | $-i \cos \theta$ | $i \sin \theta \sin \phi$ | 0 | $i \sin \theta e^{-i \phi}$ |
| $\uparrow, p_y$ | $i \cos \theta$ | 0 | $-i \sin \theta \cos \phi$ | $-i \sin \theta e^{-i \phi}$ | 0 |
| $\uparrow, p_z$ | $-i \sin \theta \sin \phi$ | $i \sin \theta \cos \phi$ | 0 | $-[(1 - \cos \theta) e^{-i \phi} + (1 + \cos \theta)]/2$ | $i -[(1 - \cos \theta) e^{-i \phi} + (1 + \cos \theta)]/2$ |
| $\downarrow, p_x$ | 0 | $i \sin \theta e^{i \phi}$ | $-[(1 - \cos \theta) e^{i \phi} + (1 + \cos \theta)]/2$ | 0 | $-i \sin \theta \sin \phi$ |
| $\downarrow, p_y$ | $-i \sin \theta e^{i \phi}$ | 0 | $-i[(1 - \cos \theta) e^{i \phi} + (1 + \cos \theta)]/2$ | $-i \cos \theta$ | 0 | $i \sin \theta \cos \phi$ |
| $\downarrow, p_z$ | $[(1 - \cos \theta) e^{i \phi} + (1 + \cos \theta)]/2$ | $i -[(1 - \cos \theta) e^{i \phi} + (1 + \cos \theta)]/2$ | 0 | $i \sin \theta \sin \phi$ | $-i \sin \theta \cos \phi$ | 0 |

The band structures of AFMz and AFMx MnBi$_2$Te$_4$ are shown in figures 1(b) and (e). The band structure is double degenerate for each $k$ point because of the coexistence of the inversion symmetry $P$ and the $S$ symmetry. We also can see that both band structures are gapped. The band gap of AFMx MnBi$_2$Te$_4$ is a little smaller than that of AFMz MnBi$_2$Te$_4$. The density of states (DOS) and projected DOS (PDOS) of Mn-$d$, Bi-$p$, and Te-$p$ orbitals for AFMz and AFMx MnBi$_2$Te$_4$ have no obvious difference, shown in figures 1(c) and (f). The occupied and unoccupied states of Mn-$d$ orbitals are far away from the Fermi level and the states near the Fermi level mainly come from Bi-$p$ and Te-$p$ orbitals.

3. The Hamiltonian with different surface magnetizations

To obtain the Hamiltonian with different surface magnetizations, we perform a self-consistent $ab initio$ calculations as a pre-process. It is worth noting that we do not consider spin–orbit coupling (SOC) in the initial self-consistent calculations in order to do with the surface magnetization. The self-consistent $ab initio$ calculations are performed in the framework of density functional theory (DFT) [35, 36] using the Vienna $ab initio$ simulation package with the plane-wave pseudo-potential method [37, 38]. Local-density approximation (LDA) is used for the exchange–correlation potential. To guarantee the convergence, the kinetic energy cutoff is fixed to 450 eV, and the $k$-point mesh is taken as Γ-centered $8 \times 8 \times 1$ for bulk calculations. The experimental lattice constants of MnBi$_2$Te$_4$ are used and atomic positions are fully relaxed until the atomic force on each atom is less than $10^{-2}$ eV Å$^{-1}$. To including the Coulomb interaction of Mn atoms, LDA + $U$ functional with $U = 3$ eV is taken. After the self-consistent $ab initio$ calculations, the charge density is fixed and a $8 \times 8 \times 3$ grid is used to obtain the maximally localized Wannier functions projected with Mn-3$d$, Bi-6$p$, Te-5$p$ orbitals [39, 40], and then we can obtain a MLWF-based TB Hamiltonian $H^T$ without SOC.

3.1. The SOC

The SOC plays a key role for the topological properties of MnBi$_2$Te$_4$ because of both the strong SOC and the magnetism, so the SOC has to be considered for our calculations. In order to conveniently tune the surface magnetization with the fixed AFMz state in the bulk, we introduce the SOC in the non-self-consistent manner. Here, we take the local atomic SOC and ignore the high-order $k$-dependence term.

The total Hamiltonian is

$$H^{tot}(k) = H^{W}(k) + H^{soc}$$

with

$$H^{soc} = \langle h/4\pi e^2 \rangle [\nabla \times \mathbf{P}] \cdot \mathbf{S},$$

where $\mathbf{V}$ and $\mathbf{S}$ represent total potential and Pauli spin matrices. The SOC term $H^{soc}$ can be written more simply as follows

$$H^{soc} = \lambda \mathbf{L} \cdot \mathbf{S},$$

where $\lambda$ denotes the SOC constant. The SOC effect of Mn atom is tiny ($\lambda_{Mn} = 0.04$ eV) [41], which is ignored in this work, and we only need to consider the local atomic SOC of Bi-$p$ and Te-$p$ orbitals. The SOC constants of Bi, Te atoms are set according to Wittel’s spectral data ($\lambda_{Bi} = 1.25$ eV, $\lambda_{Te} = 0.49$ eV) [42]. Under the basis order $\{ |p_x, \uparrow\rangle, |p_y, \uparrow\rangle, |p_z, \uparrow\rangle, |p_x, \downarrow\rangle, |p_y, \downarrow\rangle, |p_z, \downarrow\rangle \}$, we can write down the SOC term $H^{soc}$.
for $p$ orbitals with respect to spin states in direction $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ as it is shown in table 1, where the angles $\theta$ and $\phi$ are the angular spherical coordinates describing the direction of the spin quantization axis. After obtaining the Hamiltonian $H^{tot}(k)$ with the SOC effect, we calculate the bulk band structures and the surface states for bulk AFMz and AFMx MnBi$_2$Te$_4$, which agree well with DFT calculations, shown in the supplementary materials (https://stacks.iop.org/NJP/24/073034/mmedia). In addition, we calculated the Wannier charge centers (WCCs) for the Brillouin zone plane with $S^z = -1$. The WCCs show the topological invariant $Z_2 = 1$ for both AFMx and AFMz MnBi$_2$Te$_4$. Therefore, our TB model can well reproduce DFT calculations not only for the bands but also for the wavefunctions, which indicates the reliability of our TB model.

### 3.2. Surface magnetization

Once the MLWF-based TB Hamiltonian $H^{tot}$ is obtained, we can construct a semi-infinite system with different surface magnetizations. The semi-infinite system is schematically shown in figures 2(b) and 3(b). In our calculations, the topmost two SLs of MnBi$_2$Te$_4$ are taken for the surface part, and the remaining part is for the bulk. Because the local atomic SOC is considered, the SOC effect does not affect the hopping between SLs. According to table 1, the SOC term $H^{soc}$ can be written for the surface and bulk part, respectively, in accordance with the magnetic state with the spin moment in the direction $\hat{n}$. Then the surface states can be calculated using the iterative Green’s function method [43], employed in WannierTools package [44].

### 4. Tuning surface magnetizations

At first, the surface magnetization is taken as the same with the bulk magnetic ground state AFMz, shown in figure 2(b). The calculated surface states on the (111) plane is consistent with previous $ab\ initio$ calculations [18], shown in figure 2(a). Due to breaking the $S$ symmetry in the (111) surface, the surface
states are gapped, which can be simply understood due to the surface magnetization. Without the magnetism, the topological surface states of MnBi₂Te₄ can be effectively described by the Hamiltonian

\[ H_0(k_x, k_y) = \alpha_1 (k_x \sigma_y - k_y \sigma_x), \]

where \( \alpha_1 \) is the Fermi velocity. The magnetic moment of surface Mn atoms makes the magnetic exchange interaction in surface states with a mass term, and we have the Hamiltonian,

\[ H(k_x, k_y) = \alpha_1 (k_x \sigma_y - k_y \sigma_x) + m \cdot \sigma, \]

where \( m = \Delta \hat{n} = \Delta (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \) and \( \sigma \) denotes Pauli matrices. \( \Delta \) denotes the exchange field and \( \theta(\phi) \) is the polar (azimuthal) angle, indicating the magnetization direction. For the Hamiltonian \( H(k_x, k_y) \) in equation (4), we only consider the linear terms for the bands close to \( \Gamma \) point, and the high-order terms are ignored. The effects of the high-order terms are discussed in the supplementary materials. When the surface magnetization is AFMz with \( (\theta = 0, \phi = 0) \), only the \( z \)-component of \( m \) is left.

The eigenvalues are given as

\[ E(k_x, k_y) = \pm \sqrt{\alpha_1^2 (k_x^2 + k_y^2) + \Delta^2}. \]

We can see that the minimum gap is \( 2\Delta \) at the \( \Gamma \) point.

In figure 2(a), we pick two energy levels \( E_0, E_1 \) to show the FSs with the spin texture and the QPIs. In figures 2(c) and (d), the FSs of surface states corresponding to \( E_0, E_1 \) clearly present a triangle shape, indicating the \( C_{3z} \) symmetry, while the FSs of bulk states present a hexagonal shape because of the \( S \) symmetry preserved in the bulk. The spin texture presents a \( \pi \) phase. The QPIs are calculated through the joint density of states method [45] and shown in figures 2(e) and (f). We notice that though the surface states have the \( C_{3z} \) symmetry, the QPIs presents a hexagonal shape, not a triangle shape.

Secondly, the in-plane surface magnetization is studied, shown in figure 3(b). The uppermost two SLs are considered as the surface part with the in-plane magnetization AFMx, and the lower SLs as the bulk part keep the out-of-plane magnetization AFMz. The \( (\theta = \pi/2, \phi = 0) \) is for the surface Hamiltonian, and the \( (\theta = 0, \phi = 0) \) is for the bulk Hamiltonian. The surface states show a minimal gap along the \( k_y \) direction, as seen in figure 3(a), which can be understood from the effective \( k \cdot p \) Hamiltonian. When the surface magnetization is along the \( x \) direction, the effective \( k \cdot p \) Hamiltonian becomes

\[ H(k_x, k_y) = \alpha_1 (k_x \sigma_y - k_y \sigma_x) + \Delta \sigma_z. \]

The eigenvalues are obtained as

\[ E(k_x, k_y) = \pm \sqrt{\alpha_1^2 (k_x^2 + k_y^2) + (\Delta - k_y \alpha_1)^2}. \]

It can be seen that a
gapless point should arise at the point \((k_y = \Delta/\alpha_1, k_z = 0)\) along the \(k_y\) direction. But we should mention that the surface states do not completely locate within the uppermost two SLs for TB calculations in figure 3(a). The extended surface states in the lower SLs feel the bulk AFMz magnetization, so the surface states open a minimal gap along the \(k_y\) direction. Based on this understanding, the energy gap is expected to become significantly reduced through increasing the thickness of surface AFMx layer, for example, the case of the uppermost four SLs with the AFMx surface magnetization in the supplemental materials.

We calculate the FSs with the spin texture and the QPIs of surface states with the in-plane surface magnetization AFMx. The FSs at the energy levels \(E_0\) and \(E_1\) are shown in figures 3(c) and (d). From the central position of FSs, we can see that the Dirac cone is shifted from \(\Gamma\) to \((k_x, k_y) = (0, \Delta/\alpha_1)\). Also, it is seen that the FSs are no longer triangle, because the in-plane magnetization breaks the \(C_{3z}\) symmetry on the surface. The spin texture goes along the FS and still contributes a Berry phase \(\pi\). The chirality of the spin texture changes its sign from the energy level \(E_0\) to \(E_1\) crossing the gapless energy point. Corresponding to FSs, the QPIs also do not keep the hexagonal shape, shown in figures 3(e) and (f). Therefore, the broken \(C_{3z}\) symmetry of the FSs and the QPIs indicates the in-plane surface magnetization for \(\text{MnBi}_2\text{Te}_4\), which can be used as the evidence of the possible surface magnetization in experiments.

Based on our method, we can also conveniently tune the surface magnetization, for example, the smooth rotation from the out-of-plane AFMz to the in-plane AFMx. Without losing generality, we take two sets of parameters \((\theta = \pi/6, \phi = 0)\) and \((\theta = \pi/3, \phi = 0)\) to calculate the surface states, FSs with the spin texture and the QPIs, shown in figure 4. We can see that the surface states are gapped, but the energy gap gradually reduces. The FSs change into an oval shape and the QPIs are also no longer a hexagonal shape. Based on the effective \(k \cdot p\) Hamiltonian in equation (4), ignoring the high-order terms, the eigenvalues of surface states are obtained as \(E(k_x, k_y) = \pm \sqrt{k_x^2 \alpha_1^2 + k_y^2 \alpha_1^2 + \Delta^2 - 2k_y \alpha_1 \Delta \sin \theta}\). We can see that the energy gap gradually reduces with tuning the surface magnetization from \(\theta = 0\) to \(\theta = \pi/2\). Until the in-plane magnetization \(\theta = \pi/2\), the surface states become gapless as \(E(k_x, k_y) = \pm \sqrt{\alpha_1^2 k_x^2 + (\Delta - k_x \alpha_1)^2}\). In addition, for the in-plane rotation of the surface magnetization, with \(\theta = \pi/2\) and \(\phi\) from 0 to \(2\pi\), the
eigenvalues of surface states are obtained as \( E(k_x, k_y) = \pm \sqrt{(k_x \alpha_1 + \Delta \sin \phi)^2 + (k_y \alpha_1 - \Delta \cos \phi)^2} \). It is seen that the surface states keep gapless with the in-plane rotation of the surface magnetization.

5. Conclusion

We develop an effective method to study the surface states of AFM MnBi\(_2\)Te\(_4\) with tuning the surface magnetization through combining the DFT and MLWF-based TB calculations. Our results confirm that the surface magnetization has significant effects on the surface states of MnBi\(_2\)Te\(_4\). The surface states are gapped when the surface magnetization is taken as the out-of-plane AFMz. The energy gap smoothly reduces and finally becomes almost closed with a minimal value, as the surface magnetization is tuned from the out-of-plane AFMz to the in-plane AFMx. Also we can see that the FSs and the QPIs break the C\(_3\)\(_z\) symmetry, once the surface magnetization deviates from the out-of-plane direction AFMz. Our results would be valuable for understanding the gapped and gapless topological surface states observed in recent ARPES measurements of MnBi\(_2\)Te\(_4\).

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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