Interface of topological insulator Bi$_2$Se$_3$ with As$_2$Te$_3$

Niraj Aryal$^{(1)}$ and Efstratios Manousakis$^{(1,2)}$

$^{(1)}$Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 32306-4350, USA
$^{(2)}$Department of Physics, University of Athens, Panepistimioupolis, Zografos, 157 84 Athens, Greece

E-mail: manousakis@magnet.fsu.edu

Abstract. We study the topological states which appear at the interface of the topological insulator (TI) Bi$_2$Se$_3$ with As$_2$Te$_3$ which share similar size lattice constants. A Dirac-like state (DLS) with spin-momentum correlations characteristic to an edge Dirac-like state of a TI, forms at the interface. While our parity analysis shows that one should not expect a topologically protected surface state for As$_2$Te$_3$, the interface DLS has stronger overlap with the atoms of the As$_2$Te$_3$ layers, especially slightly away from the zone center. We believe that this interface DLS is the topologically protected Bi$_2$Se$_3$ edge state which “spills” over to the As$_2$Te$_3$ layers to optimize its energy.

1. Introduction

There has been significant progress towards understanding topological states of matter due to the application of state of the art experimental tools and advanced computational/theoretical techniques. The topological insulator (TI) Bi$_2$Se$_3$ is an extensively studied system since Zhang et al.\cite{1} predicted and Hasan et al.\cite{2} verified experimentally its topological signature.

Historically utilization of new phenomena in practical electronic applications is realized through interfaces, such as, a PN junction. In addition, qualitatively different phenomena from bulk can occur and have been observed on interfaces\cite{3, 4}. Furthermore, emergence of such novel phenomena have been theoretically or computationally predicted to occur in interfaces between a TI and a different material\cite{5, 6, 7}. The “interface” of the TI with vacuum, i.e., the TI surface, has been thoroughly studied and rather well understood \cite{8}. While there have been recent studies of the interfacial states formed between a TI and different types of materials, such as, band insulators (e.g., hexagonal Boron-Nitride) \cite{9}, semiconductors (e.g., GaAs) \cite{10}, graphene\cite{11, 12}, etc, our understanding is still nascent to be able to make a device for a practical purpose.

In the present paper, we consider the interface formed between the topological insulator Bi$_2$Se$_3$ (BS) and As$_2$Te$_3$ (AT), as illustrated in Fig. 1(a). The As$_2$Te$_3$ lattice structure is that of the TI family of Bi$_2$Se$_3$ and Bi$_2$Te$_3$. Furthermore, the lattice constant of AT is 4.089 Å which is close to that of BS (4.14 Å). Therefore, it looks promising that one can realize such an interface in practice. Unlike BS, in AT the weak spin-orbit coupling due to As atoms is not enough to cause an inversion at the valence and conduction bands near the Γ point and, hence, AT is not topological which is confirmed by our parity analysis using the recipe of Ref. \cite{13}. We would
like to investigate, as a function of the number of layers, the formation or lack of formation of a topological interface state and to characterize it.

Figure 1. (a): The slab which was used in our calculations. (b),(c), and (d): The band structure obtained for various structures. See text for details.

2. Computational details

The calculations presented here are carried out using the Quantum Espresso[14] implementation of the density functional theory (DFT) in the GGA framework including spin-orbit coupling (SOC). The Perdew-Burke-Ernzerhof (PBE) exchange correlation functional[15] was used with fully relativistic PAW pseudo-potentials[16].

The plane-wave energy cutoff was taken to be 80 Ry and a \( k \)-point mesh of \( 15 \times 15 \times 1 \) was used. The slab calculation of the pristine Bi\(_2\)Se\(_3\) was done using 5 quintuple layers (QLs) whereas the interface calculation was done using 5 and 6 QL of BS with 1 QL of AT on both sides of the slab. A vacuum layer of \( 17-20 \) Å was placed to avoid interaction between the periodic images.

We will consider two structures: (a) Structure S1: an AT/BS/AT structure in which we use 5 QLs of Bi\(_2\)Se\(_3\) and 1 QL of As\(_2\)Te\(_3\) on each surface of the Bi\(_2\)Se\(_3\) slab. (b) Structure S2: an AT/BS/AT structure in which we use 6 QLs of Bi\(_2\)Se\(_3\) and 1 QL of As\(_2\)Te\(_3\) on each surface of the Bi\(_2\)Se\(_3\) slab.

Figure 2. Total sum of the projections of all interface Dirac-like states at the \( \Gamma \) point onto the atomic wavefunction of each layer.
3. Band structure

Our calculated bands for a slab illustrated in Fig. 1(a), which consists of 1QL-AT/5QL-BST/1QL-AT (which we will refer to as structure S1), are presented in Fig. 1(b). The bands obtained for the same structure as in Fig. 1(a) using 6 BS QLs (which we will refer to as structure S2) are shown in Fig. 1(c). For comparison the band structure of a slab which consists of 5 QLs of pure BS is also presented in Fig. 1(d). In all cases the gray ribbons are the 3D bands of pure crystal BS projected on the a-b plane. First, notice that in the case of the pure slab the bulk ribbons overlap with the states of the slab, except for the Dirac cone which forms in the bulk gap at the Γ point. This topologically protected Dirac-like state which appears for a slab of pure BS has been well-studied previously [8, 1] For the case of Figs. 1(b,c) we shifted all the bands of the slab by a constant energy value equal to the difference between the energy of the bulk ribbons far away from the Fermi level and the energy of the corresponding slab states. Notice that if we do that, the bulk ribbons overlap with the slab states even near the Fermi level and this provides a good guide to the eye for what happens. In Figs. 1(b,c) we denote the slab Fermi level by $E_F^{(S)}$ and the BS bulk Fermi level by $E_F^{(B)}$.

Notice that when we use 6 QLs of BS in the AT/BS/AT interface structure (S2 structure) a Dirac-like surface state forms in the bulk BS gap. As will show later, this state is an interface state and is also characterized by the spin-momentum correlations for an edge state of TI. In the S1 structure (5 BS QLs), there is a small gap separating the top and bottom Dirac cones.

4. Nature of the interface bands

Fig. 2 illustrates the degree of localization near the surface of the Dirac-like states (DLS). Notice that in the case of the S2 structure, the DLS are mainly localized near the interface (Fig. 2(b)) with almost zero contribution from the “bulk” layers, i.e., there are layers away from both interfaces with negligible contribution to the DLS, just like in the pristine BS slab case shown in Fig. 2(c). However, in the case of the S1 structure, the DLS are not just localized near the interface layers (Fig. 2(a)) as their wavefunctions has significant overlap with the atoms of all the layers in the 5 QLs of BS. Namely, the DLS wavefunctions are characterized by a width which is greater than half the size of our BS slab. We believe that this is the reason of the opening of the gap between the upper and lower DLS seen in Fig. 1(b). Therefore, we conclude that a slab with number of QLs greater or equal to 6, is large enough to yield gapless DLS at the interface. In Figs. 3(a,b) we present the character of the bands for the S2 structure. The size of the circles used is proportional to the total projection of the interface state onto the atomic wavefunction of the atoms forming the AT QL (red circles) and the one of the BS QLs which is closer to the interface (blue circles). Notice that the wavefunctions of the DLS have a significant overlap with the atoms of the AT layers. This is also clear from Fig. 2(b) for the Γ point. The contribution of the AT layers becomes greater as we move away from the Γ point.

![Figure 3](image-url). Contribution of the AT layers ((a), red circles) and of the BS layers ((b), blue circles) to DLS. (c) $\langle \sigma_x \rangle$ along $k_y$ and (d) $\langle \sigma_y \rangle$ along $k_x$ for the interface Dirac-like states.
5. Spin-momentum correlations of the interface bands
The spin-momentum correlation of a pure BS slab has been calculated by Yazyev et al. [17]. In Figs. 3 (c,d) we present the results of our calculations of the spin-momentum correlations for the 1QL AT/6QLs BS/1QL AT system considered in the present paper. We have labeled the curves as $X\nu$ where $X=U,L$, stands for the upper and lower branches of the Dirac cone and $\nu = 1,2$, stands for the top and bottom surface of the lab. Notice that the expectation value of $\sigma_x$ along the $k_x$ direction is zero while along the $k_y$ is significant and the upper and lower branch of the Dirac cone are characterized by opposite relative spin orientation and similarly the same branches of the Dirac cone which belong to the top or bottom surface of the slab have opposite spin correlation.

6. Conclusions
We have studied the interface of the topological insulator Bi$_2$Se$_3$ (BS) with a single quintuple layer of As$_2$Te$_3$ (AT) and we varied the size of the Bi$_2$Se$_3$ slab. We find that a Dirac-like cone forms inside the bulk BS band gap and its physical location, when the BS slab is large enough, is at the interface. We find that the wavefunction of this interface state has a significant extension inside the AT layer. In fact, we find that as we move away from the $\Gamma$ point, most of the wavefunction of the interface Dirac-like cone lies inside the AT layer. When the number of QLs of BS is 5, the interface Dirac-like state has overlap with every atom of the BS slab, because of the interaction between the two interfaces which are close. In this case the interface Dirac-like cones have a gap. When the number of QLs in the BS slab is 6, we find that the two Dirac-like interface states which form on both interfaces are separated by a spatial gap where their wavefunction is negligible. Therefore, when the thickness of the BS slab is greater or equal to 6 QLs, the Dirac-like interface states are localized at the interfaces. In this case the Dirac cones are gapless. We also calculated the spin-momentum correlations of these interface Dirac-like states and we found that they are the same to those of the topologically protected surface states of the topological insulator.

7. Acknowledgments
This work was supported in part by the U.S. National High Magnetic Field Laboratory, which is funded by NSF DMR-1157490 and the State of Florida.

8. References
[1] Zhang H, Liu C X, Qi X L, Dai X, Fang Z and Zhang S C 2009 Nature physics 5 438–442
[2] Xia Y, Qian D, Hsieh D, Wray L, Pal A, Lin H, Bansil A, Grauer D, Hor Y, Cava R et al. 2009 Nature Physics 5 398–402
[3] Cen C, Thiel S, Hammerl G, Schneider C W, Andersen K E, Hellberg C S, Mannhart J and Levy J 2008 Nat. Matt. 7 278–302
[4] Okamoto S and Millis A J 2004 Nature 428 630
[5] Fu L and Kane C L 2008 Phys. Rev. Lett. 100 096407
[6] Teo J C Y and Kane C L a 2010 Phys. Rev. B 82 115120
[7] Zhang Q, Zhang Z, Zhu Z, Schwingenschlgl U and Cui Y 2012 ACS Nano 6 2345–2352
[8] Hasan M Z and Kane C L 2010 Rev. Mod. Phys. 82(4) 3045–3067
[9] Jin H, Im J, Song J H and Freeman A J 2012 Phys. Rev. B 85(4) 045307
[10] Seixas L, West D, Fazzio A and Zhang S B 2015 Nature Communications 6 7630 EP – article
[11] Zhang J, Triola C and Rossi F 2014 Phys. Rev. Lett. 112 096802
[12] Spatarn C D and Léonard F n c 2014 Phys. Rev. B 90(8) 085115
[13] Fu L and Kane C L 2007 Phys. Rev. B 76(4) 045302
[14] Giannozzi P, Baroni S, Bonini N, Calandra M, Car R, Cavazzoni C, Ceresoli D and et al 2009 Journal of Physics: Condensed Matter 21 395502 (19pp)
[15] Perdew J P, Burke K and Ernzerhof M 1996 Phys. Rev. Lett. 77(18) 3865–3868
[16] Blöchl P E 1994 Phys. Rev. B 50(24) 17953–17979
[17] Yazyev O V, Moore J E and Louie S G 2010 Phys. Rev. Lett. 105(26) 266805