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Strain-driven tunable topological states in Bi$_2$Se$_3$

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Abstract

Strain allows to manipulate the topological phase and to induce a topological phase transition (TPT) in three-dimensional Bi-chalcogenide topological insulators. Here we propose the formation of strain-driven topological homojunctions (THs) in Bi$_2$Se$_3$. By applying inhomogeneous tensile strain to a film of Bi$_2$Se$_3$ a TPT is induced inside the film, and in this way a TH containing topological and trivial Bi$_2$Se$_3$ phases is formed. Based on first principles calculations we demonstrate that topological states can be created and destroyed in Bi$_2$Se$_3$ systems containing one or more homojunctions and show how the spatial localization and doping of topological interface states, arising within Bi$_2$Se$_3$ THs, can be reversibly tuned. This type of homojunctions is the simplest topological interface and thus constitutes the ‘Hydrogen atom’ of topological states of matter. Our findings show a route to tune and manipulate topological states by strain and are promising to be exploited in topological devices.

1. Introduction

Strain engineering has been used for several decades to tune and optimize the physical properties of a variety of materials, from traditional bulk semiconductors to complex oxide heterostructures. The band structure of a material can be modified by strain, and thus it is a powerful tool to tailor distinct properties, which could be useful for the development of new functionalities and novel devices. Strain has also been proposed as an effective mechanism to drive a topological phase transition (TPT) in the recently discovered topological insulators (TIs). This novel phase of matter is fundamentally distinct from non-topological materials because it can not be ascribed to a spontaneous symmetry rupture. Instead, topological phases are correctly described by topological invariants [1–5]. In the last few years, topology has been found to play an essential role in defining many phases of matter such as the quantum Hall effect [1], the quantum spin–Hall effect [6, 7], the quantum anomalous Hall effect [8, 9], Weyl semimetals [10–12] or topological nodal line semimetals [13–15] to mention just a few. Specifically, Bi-chalcogenide three-dimensional TIs are characterized by a non-zero $\mathbb{Z}_2$ topological invariant, and according to the bulk-to-boundary correspondence [5, 16], they exhibit topological states at the boundary with any material with a different value of the topological invariant. In particular, Bi-chalcogenide TIs host gapless surface states that are topologically protected by time-reversal symmetry. These materials have an insulating gap in the bulk, while the electrons at the surface (i.e. at an interface with vacuum) resemble massless helical Dirac fermions, with spin locked to the crystal momentum [17, 18]. Topological surface states (TSSs) in Bi-chalcogenide TIs have been extensively studied, both theoretically and experimentally, since these compounds are of particular interest due to their relatively large gaps and single Dirac cone at the center of the Brillouin zone (BZ). They are very promising for spintronics and low power consumption electronics as well as for emerging properties and novel functionalities.

In the Bi$_2$Se$_3$ family of compounds (Bi$_2$Te$_3$, Sb$_2$Te$_3$, Bi$_2$Se$_3$, and Sb$_2$Se$_3$) the topological insulating phase results from inversion of the band gap, due to the strong spin–orbit coupling (SOC), at the time-reversal invariant $\Gamma$ point of the BZ. Several works have assessed the importance of strain in these materials and its influence on their topological order. The bulk band topology has been predicted to be sensitive to strain, since the latter can strongly affect the inverted gap. In fact, the transition from the topological to the trivial phase was predicted to occur for these bulk materials under purely uniaxial strain [19–25]. In a recent work, we
investigated the combined effect of both uniaxial and biaxial strain on the topology of the Bi$_2$Se$_3$ family and found a universal phase diagram [26]. All the compounds can exhibit metallic and insulating phases, both topologically trivial and non-trivial, and uniaxial tensile strain applied in the (0001) direction triggers a TPT, the critical strain being compound dependent.

It has been demonstrated that TSSs can be tuned at grain boundaries in Bi$_2$Se$_3$ (0001) films [27, 28]. Experiments show that alternating edge dislocation pairs along the boundary introduce periodic in-plane tensile and compressive strains, which in turn shift the energy of the Dirac state and open a gap [28]. Also, strain-induced reversible Fermi level tuning in Sb$_2$Te$_3$ films [29] and Dirac state shifts in single-crystal Bi$_2$Se$_3$ nanowires bent by an external force have been reported [30]. Furthermore, recent studies point to the feasibility to induce controllable strain either in thin films or 2D structures. Strained structures of a single material such as Bi$_2$Se$_3$ films [16], layered structures containing two compounds such as Bi$_2$Te$_3$/Sb$_2$Te$_3$ [31] and Bi$_2$Se$_3$/In$_2$Se [22] or even Bi$_2$Se$_3$/$\text{Bi}_2\text{Te}_3$ lateral heterojunctions with a large lattice mismatch [32] have been synthesized. In these strained structures either uniform strain or a strain gradient is achieved.

Motivated by our previous work and the recent experimental advances, here we propose a feasible mechanism to reversibly switch topological states inside films of Bi-chalcogenides. We demonstrate that by applying a simple uniaxial stretch to both ends of a (0001) Bi$_2$Se$_3$ slab, elastic deformation will induce an expansion of the lattice along the (0001) stretching direction, while the six-fold rotational invariance is preserved. This results in a non-uniform uniaxial tensile strain perpendicular to the cell with non-zero lattice parameter to its equilibrium value $a = 4.17$ Å, tantamount to a real space grid resolution below 0.05 Å$^{-1}$.

The slabs and superlattices (SLs) were built using the bulk atomic positions and out-of-plane lattice parameters (the particular values are specified in each case). The electronic structure DFT calculations for the slab and SL systems were obtained using the SIESTA [34] code, through its implementation in the GREEN package [35]. We employed the Perdew–Burke–Ernzerhof [36] generalized gradient approximation in all calculations. Weak van der Waals (vdW) interactions between quintuple layers (QLs) were accounted for within the semi-empirical pair-potential vdW correction of Grimme [37] as implemented in the VASP code. BZ integrations were performed on Monkhorst-Pack $k$-point meshes of 13 × 13 × 1 for slabs and SLs, and of 13 × 13 × 13 for bulk systems. The energy cut-off was set to 340 eV for the plane wave basis set in VASP calculations, and a double $\zeta$-polarized scheme with confinement energies of 100 meV was used for the numerical orbital basis set in SIESTA. The three-center integrals appearing in the SIESTA formalism were calculated using an hyperfine mesh cut-off of 1200 Ry, tantamount to a real space grid resolution below 0.05 Å$^{-1}$. The SOC was included in all calculations in a self-consistent manner [38, 39].

Bismuth selenide shows a rhombohedral crystal structure belonging to spatial group $R3m$ ($D_3^5$). The unit cell consists of 5 consecutive atoms Se–Bi–Se–Bi–Se that follow an ABCABC... stacking sequence [17, 18], which forms a so-called QL (see figure 2). The system shows strong chemical bonding between adjacent layers within the QL, while the inter-QL coupling is of the weak vdW kind.

The effect of uniaxial strain on bulk Bi$_2$Se$_3$ has been addressed in a previous work [26] and is summarized in figure 1. Tensile strain along the (0001) direction shifts the Se (Bi) $p_z$ bands around the $\Gamma$ point towards lower (higher) energies, eventually leading to a band un inversion. In this process the system undergoes a TPT from a TI with non-zero $Z_2$ index to a normal insulator (NI) with zero $Z_2$ index. The critical strain is found to be 6.3%, corresponding to an out-of-plane lattice vector of $c = 30.2$ Å, at which the bulk band gap closes — see figure 1(e) —. In this article we exploit this idea to build topological homojunctions (THJs), i.e., junctions composed of the same material in different topological phases. In all the systems discussed in this work we have fixed the in-plane lattice parameter to its equilibrium value $a = 4.17$ Å [26], and the stacking sequence of the ideal bulk is maintained in all cases throughout the homojunctions. The vdW gap between two QLs with different strain values is taken as the average vdW gap of the two subsystems. In the inversion asymmetric slabs dipole corrections were included in the calculations along the (0001) direction in order to avoid spurious electrostatic interactions among periodic images of the system [40].

2. Methods and crystal structure

We performed density functional theory (DFT) calculations in order to obtain the atomic and electronic structure of the different systems studied. For the bulk structures, we fixed the in-plane lattice parameter to its equilibrium value ($a = 4.17$ Å) and we varied the value of the lattice parameter $c$. The atomic positions for each bulk structure were allowed to relax using the VASP code [33] until forces became smaller than 0.01 eV Å$^{-1}$.

Corrections were included in the calculations along the $\zeta$ direction shifts the Se–Bi–Se–Bi–Se that follow an ABCABC... stacking sequence [17, 18] which forms a so-called QL (see figure 2). The system shows strong chemical bonding between adjacent layers within the QL while the inter-QL coupling is of the weak vdW kind.

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3. Bi$_2$Se$_3$ (0001) thin films under a strain gradient

We first consider a Bi$_2$Se$_3$ (0001) thin film under equal uniaxial stretch forces applied on the opposite surfaces. In the elastic regime the stretching yields a gradient of internal stress decaying towards the center of the film. Thus, we model the system by imposing a gradually increasing tension along the (0001) direction, from the center towards the surfaces, to a 13% Bi$_2$Se$_3$ film—see figure 2(a)—. The film is symmetric with respect to the central QL and the corresponding out-of-plane lattice parameter changes linearly from 28.4 Å in the central QL to 32.0 Å at the surface QL. Hence, the central QL is kept unstrained, while the external QLs show a 12% tensile strain, which is twice the critical strain needed for the TPT in Bi$_2$Se$_3$. Thereby, the slab shows a constant strain gradient and fulfills overall inversion symmetry by construction. In a real sample, due to the weak vdW interaction between QLs, a more complex strain distribution profile along the (0001) direction is expected. Nevertheless, our results should hold since the TPT will necessarily take place as long as the critical strain (6.3% in Bi$_2$Se$_3$) is reached. The strained film equals a double TH between two semiconductors in the NI phase and TI phase, respectively, i.e. a NI/TI/NI homojunction. The interfaces lay within the film at the fourth QLs from the surfaces, which present the critical strain—they are marked as shaded regions in figures 2(c) and (d)—. The bulk-to-boundary correspondence dictates that a topological state must arise at the interfaces. This is indeed
what we find. The electronic structure of the thin film around the center of the BZ is shown in figure 2(b). The linear dispersion of the Dirac cone TIS is almost isotropic around \( \overline{G} \), being the constant energy contours circular. Hence the velocity of the topological interface electrons is practically independent of the direction. The layer projected density of states (LDOS) of the Dirac states is shown in figures 2(c) and 2(d). We see that the topological states are localized at the interface between the TI and the NI phases of Bi\(_2\)Se\(_3\) and expand around four QLs. Note that the TISs are two-fold degenerate due to inversion symmetry, and each member of the degenerate pair is localized at a different interface. In the figure we show the LDOS profile of both TISs in each case. The spin texture for one of the degenerate TISs is shown in figure 2(e)—above the Dirac point—and (f)—below the Dirac point. The arrows correspond to the expectation value for the spin at each \( k \)-point, while the \( S_z \) component is additionally color coded according to the scale shown at the right of the figure. The maximum value \( S_z \) achieves is \( \pm 30\% \) of the modulus of the total spin \( S = \sqrt{S_x^2 + S_y^2 + S_z^2} \).

Figure 2. Bi\(_2\)Se\(_3\) topological homojunction slab with strain gradient along the (0001) direction. The electronic structure of the system is shown in (b), and the local density of states of the electron-like and hole-like topological interface states (marked with colored points in the band dispersion diagrams) are shown in (c) and (d), respectively. The TISs are two-fold degenerate, and the LDOS profile for both degenerate states is shown in each case. The spin texture of one of the TISs is shown in (e)—electron-like TIS, above the Dirac point—and (f)—hole-like TIS, below the Dirac point. The arrows correspond to the expectation value for the spin at each \( k \)-point, while the \( S_z \) component is additionally color coded according to the scale shown at the right of the figure. The maximum value \( S_z \) achieves is \( \pm 30\% \) of the modulus of the total spin \( S = \sqrt{S_x^2 + S_y^2 + S_z^2} \).

In order to check the experimental feasibility of our proposal, we analyse the stability of the strained film under exfoliation. We estimate the exfoliation energy of the surface QL, which is under the largest strain considered, as the difference between the energy per surface unit area of the full strained slab and that of the two isolated subsystems (one composed by the first 12 QLs and the other composed by only the surface QL). The difference is 13.0 meV Å\(^{-2}\), of the same order as 22.4 meV Å\(^{-2}\), previously reported for the exfoliation energy of unstrained Bi\(_2\)Se\(_3\) [18, 41]. This analogy between the TIS and TSS is due to the fact that although the strain is inhomogeneous in the out-of-plane direction, the in-plane rotational symmetry of the lattice is preserved. For strained films with broken in-plane rotational symmetry, the Dirac cone becomes anisotropic [25].

In order to check the experimental feasibility of our proposal, we analyse the stability of the strained film under exfoliation. We estimate the exfoliation energy of the surface QL, which is under the largest strain considered, as the difference between the energy per surface unit area of the full strained slab and that of the two isolated subsystems (one composed by the first 12 QLs and the other composed by only the surface QL). The difference is 13.0 meV Å\(^{-2}\), of the same order as 22.4 meV Å\(^{-2}\), previously reported for the exfoliation energy of unstrained Bi\(_2\)Se\(_3\) [42]. On the other hand, the energy per surface unit area required to expand Bi\(_2\)Se\(_3\) along the (0001) direction up to a 12.7% strain is obtained as the energy difference between the unstrained bulk and that of the bulk with \( c = 32.0 \) Å, divided by the surface area. This calculation yields a value of 5.2 meV Å\(^{-2}\), which is less than half of the estimated exfoliation energy for the last QL. Therefore, the system will remain bounded upon applying up to at least 12.7% tensile strain.
4. THs with a step-like strain profile

In order to investigate the properties of the strain-induced topological states, we now build Bi$_2$Se$_3$ THs composed of only two distinct types of subsystems: unstrained Bi$_2$Se$_3$ ($c = 28.4 \text{ Å}$, TI), and Bi$_2$Se$_3$ under a uniaxial tensile strain of 12.7% ($c = 32.0 \text{ Å}$, NI) (see figure 1 first and third row, respectively). Both systems show a bulk band gap of ±0.3 eV, the plus (minus) sign corresponding to the NI (TI) phase. First we focus on SLs composed of $n$ QLs of NI and $m$ QLs of TI ($n/m$ SLs) and vary either $n$ or $m$ independently. The electronic structure of the 6/6 SL is shown at the top of figure 3. TISs arise at both interfaces, yielding two-fold degenerate Dirac cone-like states. They are localized around the interface between the NI and TI subsystems, with a slightly larger weight on the TI side. When the thickness of the TI layer is decreased to $m = 2$ and 1 QLs—figures 3(e) and (f), respectively—the two opposite interfaces are brought closer together and a hybridization gap opens up in the band spectrum. The gap is as large as 135 meV for the system with a single TI QL. The TIS–TIS hybridization is similar to the TSS–TSS coupling found in TI thin films [26, 43]. If we instead keep the thickness of the TI subsystem fixed to $m = 6$ QLs and decrease the thickness of the NI to $n = 2$ and 1 QLs—figures 3(h) and (i), respectively—we find that a gap is also opened. For the thinnest thickness of the NI subsystem (1/6 SL), the gap is of 106 meV, slightly smaller than in the 6/1 SL discussed above. All the SLs shown in figure 3 are inversion symmetric by construction, and therefore the TISs are doubly degenerate. In the LDOS profiles displayed in figures 3(a)–(c) and (j)–(l) we show both TISs in different colors. The appearance of the hybridization gap induces an effective mass in the interface electrons, which is associated with the increase of the $S_z$ component of the spin expectation value. Note that the evolution of the TIS with the thickness of both the TI or the NI is analogous, with a slightly larger gap for the thinnest TI SL.

We also build inversion symmetric films with the structure TI/NI/TI and different thicknesses of the TI layer on both sides. They can be obtained by truncating the SLs shown in figure 3 at the center of the TI slab. In figure 4 we show the evolution of the electronic structure and LDOS of such films with a NI central layer of 6 QLs and TI layers on both sides of 3, 2 and 1 QLs for panels (d), (e) and (f), respectively. In all the cases the system hosts two degenerate TISs and two degenerate TSSs (localized on opposite interfaces and surfaces, respectively). For thicknesses of the TI layers below 3 QLs, the NI/TI interface and the surface are close enough for the TIS and the TSS to hybridize. The TIS–TSS coupling is largest for the slab with only 1 TI QL on the sides, in which the LDOS profile of the TIS and that of the TSS are almost identical—see figure 4(c)—. This hybridization leads to a gap opening, which becomes as large as 194 meV for the thin film with the thinnest TI layer. Note that this value is almost 50% larger than the hybridization gap of the TIS 6/1 SL. Moreover, although the structure presents a global inversion symmetry, the local asymmetry between the surfaces and the interfaces induces a Rashba-like splitting of the topological states. The Dirac point of the TISs (TSSs) is slightly above (below) the Fermi energy.
due to the structure inversion asymmetry. However, because of the global inversion symmetry, the bulk-like bands localized within the film are not Rashba--split (see the bands above the topological states in figure 4).

5. Asymmetric topological junctions: strain dependence

All the results reported above correspond to structures with an inversion center. We finally investigate the thickness and strain dependence on inversion symmetry breaking Bi$_2$Se$_3$ thin films. To this end, we first build asymmetric thin films with a single topological junction, composed of a 4 QL thick slab of Bi$_2$Se$_3$ in the NI phase with $c = 32.0$ Å and a Bi$_2$Se$_3$ slab in the unstrained TI phase ($c = 28.4$ Å). We vary the thickness of the TI layer, always keeping it above 3 QLs so that the TIS and the TSS are spatially separated and thus decoupled. The results are shown in figures 5(a)–(c) for a TI thickness of 4, 6, and 8 QLs, respectively. These films can be compared with the symmetric slab shown on the first row of figure 4. The splitting between the TIS and the TSS is now much smaller, almost negligible, and there is a slight n-doping of the topological states that increases with the number of TI QLs. Furthermore, in the three films all the bands (including the bulk-like ones) are
Rashba–split, as expected from the global asymmetry of the film, and in contrast to the inversion-symmetric systems discussed in the previous section. Reducing the TI thickness below 4 QLs also results in a gap opening due to TSS–TIS interaction (not shown), as previously discussed for the symmetric case.

Up to this point, in all the discussed structures the uniaxial strain has been of the tensile type (positive), since it promotes the TPT. Nevertheless, compressive uniaxial strain also affects the topological states. The Dirac point shifts to lower energies under compression [26]. Thus, for comparison, we compute similar inversion asymmetric thin films in which the TI subsystem is now under 4.9% compressive uniaxial strain (instead of unstrained as in the previous case), corresponding to an out-of-plane lattice parameter of $c = 27.0$ Å. The electronic structure of these thin films is displayed in figures 5(d)–(f). The TSS–TIS splitting is very large and the TSS becomes notoriously n-doped, while the TIS is only slightly n-doped in all cases. Increasing the size of the TI layer enhances the TSS doping. There is also a Rashba splitting of all the bands, being larger for the topological states than for the bulk-like bands. These findings prove that the doping of the TSSs in THs can be tuned by means of uniaxial strain [26].

6. Summary and conclusions

By strain engineering we have proposed and built several THs based on Bi$_2$Se$_3$. We first mimic a realistic and feasible scenario in which tensile strain is applied gradually from the ends (either mechanically or chemically [44]) of a Bi$_2$Se$_3$ TI film. Upon applying strain from the ends of the film, topological states emerge at the interfaces between the TI and NI subsystems, once the strain reaches and overcomes the critical value. The TIS preserves the physical properties of TSSs, namely its topological protection and spin texture. Hence, we propose strain as a mechanism to tune topological states inside a film and consequently to protect them from ambient impurities or gas adsorption. We have also analyzed the dependence of the electronic structure and topological state localization with the layer thicknesses. In SLs, sufficiently thin layers of NI or TI can induce a hybridization gap between TISs, analogous to the observed TSS–TIS hybridization. In addition, in slab systems the TISs can also hybridize with the TSSs. Furthermore, applying compressive strain to the TI layer results in notorious electron doping of the TSSs. Finally, in this article we have introduced the concept of THs, which can be regarded as the ‘Hydrogen atom’ of TIs, since they host topologically protected states within two subsystems which share spatial and magnetic group as well as chemical composition, and even show an identical bulk band gap, the crucial difference between them being only their topological state. All the results discussed in this article can be generalized to the whole Bi$_2$Se$_3$ family of compounds, as well as to any other TI in which strain can drive a TPT. They also offer new opportunities to control spin currents inside TI films or multilayers and show a route to the development of strain-based topological devices.

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