Quantum spin Hall effect and topological phase transition in InN$_x$Bi$_y$Sb$_{1-x-y}$/InSb quantum wells

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Abstract

Quantum spin Hall (QSH) effect, a fundamentally new quantum state of matter and topological phase transitions are characteristics of a kind of electronic material, popularly referred to as topological insulators (TIs). TIs are similar to ordinary insulator in terms of their bulk bandgap, but have gapless conducting edge-states that are topologically protected. These edge-states are facilitated by the time-reversal symmetry and they are robust against nonmagnetic impurity scattering. Recently, the quest for new materials exhibiting non-trivial topological state of matter has been of great research interest, as TIs find applications in new electronics and spintronics and quantum-computing devices. Here, we propose and demonstrate as a proof-of-concept that QSH effect and topological phase transitions can be realized in InN$_x$Bi$_y$Sb$_{1-x-y}$/InSb semiconductor quantum wells (QWs). The simultaneous incorporation of nitrogen and bismuth in InSb is instrumental in lowering the bandgap, while inducing opposite kinds of strain to attain a near-lattice-matching conducive for lattice growth. Phase diagram for bandgap shows that as we increase the QW thickness, at a critical thickness, the electronic bandstructure switches from a normal to an inverted type. We confirm that such transition are topological phase transitions between a traditional insulator and a TI exhibiting QSH effect—by demonstrating the topologically protected edge-states using the bandstructure, edge-localized distribution of the wavefunctions and edge-state spin-momentum locking phenomenon, presence of non-zero conductance in spite of the Fermi energy lying in the bandgap window, crossover points of Landau levels in the zero-mode indicating topological band inversion in the absence of any magnetic field and presence of large Rashba spin-splitting, which is essential for spin-manipulation in TIs.

1. Introduction

Topological insulators (TIs) are a recently discovered class of electronic material that have a bulk bandgap similar to that of an ordinary insulator, but have gapless conducting states on their surface or edge that are topologically protected [1]. These topological surface states are facilitated by the time-reversal symmetry and they are robust against nonmagnetic impurity scattering [1, 2]. They have a Dirac-type energy-momentum relation, unusual spin texture with a Berry’s phase of $\pi$ and exhibit non-dissipative conduction channels that are counter-propagating and fully spin-polarized [2, 3]. In current research, TIs have been successfully realized in both two-dimensional (2D) and three-dimensional structures. In this work, we focus on the 2D TIs, which is a...
quantum spin Hall (QSH) insulator, and is closely related to the integer quantum Hall state [1]. Apart from their intriguing fundamental physical properties which has stirred a lot of research interest in the condensed-matter community recently, they are a candidate with immense potential for application in new electronic, spintronic and quantum computation devices with low power dissipation [4]—for which a new term topotronics⁷ has been newly coined [2].

In 2006, for the first time Bernevig et al [5] theoretically predicted QSH effect to exist in 2D semiconductor HgTe/CdSe quantum wells (QW) having an uniform strain gradient. It was experimentally confirmed a year later through transport experiments by König et al [6]. Thereafter, researchers paid increased attention on finding more TI materials in traditional semiconductor systems. The InAs/GaSb/AlSb Type-II QW was theoretically proposed [7] and confirmed through the transport experiments [8]. By 2009, other second-generation TIs such as Bi₂Se₃, Bi₂Te₃, and Sb₂Te₃ were experimentally identified [9]. Later, other semiconductor systems exhibiting QSH effect were proposed, such as 2D GaAs with hexagonal symmetry [10], InN/GaN QW [11] and Ge/GaAs QW [12]. He et al have recently demonstrated magnetic TIs coupled through an antiferromagnetic layer using Cr-doped (Bi, Sb)₂Te₃ [13]. InSb has also been explored theoretically, and it has been demonstrated that normal bulk InSb can be converted to exhibit a topologically nontrivial phase by inducing a biaxial lattice expansion of 2%–3% based on the density functional theory and tight-binding calculation [14]. A recent proposal design a p–n junction QW [15] to invert the band utilizing the built in electric field. Both the schemes claim that InSb is indeed a promising material to realize TIs.

Based on the aforementioned premise, in this work we propose and verify as a proof-of-concept that InₙBiₙSb₁₋ₓ₋ₓ/y/InSb QW grown along the [001] direction as a semiconductor system can effectively realize QSH effect and topological phase transition. The presence of both N and Bi doped impurities in InSb makes the band inversion easier to realize, and has a twofold advantage: (i) firstly, the conduction band (CB) edge has a negative shift (lowering of CB edge) due to N doping, while the valence band (VB) edge has a positive shift (lifting of VB edge) due to Bi doping. These two phenomenon occur simultaneously and independently of each other [16], which greatly increases the possibility of band inversion, if appropriate proportion of N and Bi were doped. (ii) Secondly, the doping of N alone induces tensile strain (ε₁ > 0), while Bi alone induces compressive strain (ε₂ < 0), both of which are a concern for lattice growth by molecular beam epitaxy or metal organic chemical vapor deposition. However, with the ideal extent of incorporating both N and Bi, we can significantly reduce the strain or even attain lattice-matching, essential for high quality material growth. Thus N- and Bi doping in InSb opens avenues for stain-engineering and bandgap-engineering simultaneously. It has been experimentally shown that, by varying the composition of N and Bi, the band gap of InₙBiₙSb₁₋ₓ₋ₓ/y can be tuned to be near zero and even negative [17, 18]. This can be theoretically explained by the band anticrossing (BAC) model [16, 19–21]. The N-related resonant states couple with the CB and lowers the CB edge [22]. Similarly, the reduction of the bandgap in InBiₙSb₁₋ₓ₋ₙ₋y, has been observed in experiments [23–26] and explained by the valence band anticrossing (VBAC) model [27]. The Bi-related resonant states couple with the VB and lifts the VB edge [27]. Therefore, the incorporation of N and Bi in InSb simultaneously offers a promising proposal to realize TIs.

The rest of the paper is organized as follows. Section 2.1 gives the 16-band k · p model which takes the effect of the resonant states induced by the N and Bi impurities into consideration. In section 2.2, we show how to derive the effective 6-band Hamiltonian using Lowding [28] perturbation method. In section 2.3, we show the method to calculate the two-terminal conductance. After description of the theoretical model, we illustrate the results of topological phase transition. In section 3.1 we witness the band inversion with increasing width of the well. In order to confirm that the above band inversion is indeed a topological phase transition, we study the bandstructure with the help of effective Hamiltonian obtained in section 3.2. Then the distribution of the wavefunctions, and the spin-momentum locking phenomena is studied in section 3.3, the edge transport properties in section 3.4 and the magnetic field effect in section 3.5. In addition, section 3.6 demonstrates the topological phase transition when the concentration of impurities is increasing. Finally, we conclude the article by establishing as a proof-of-fact that InₙBiₙSb₁₋ₓ₋ₓ/y/InSb QWs can indeed be a TI material.

2. Theoretical model and methods

2.1. 16-band k · p model

Band theory of solids is an excellent framework to study and understand TIs, wherein we use a crystal’s momentum k to classify its electronic states by exploiting the translational symmetry of the crystal within a periodic Brillouin zone [1]. The energy bands that collectively determine the electronic bandstructure can be obtained by solving for the eigenvalues of the Hamiltonian H defining the quantum mechanical system [29].

⁷ Topotronics stands for topological electronics. A recent article in Science News has cited [4] (http://scienencenews.org/article/weird-materials-could-make-faster-computers) on how TIs can enable efficient electrical manipulation of magnetic materials for memory and logic applications.
Previously, both Bernevig et al [5] and König et al [6] have used the 8-band $k \cdot p$ model and 4-band effective Hamiltonian to study HgTe/CdTe QW TIs. But in this work we propose a 16-band $k \cdot p$ model due to the presence of N and Bi in our system. In addition to to Kane’s 8-bands, we need two additional bands to incorporate the local N resonant s-like states. Moreover, we also need six additional bands to incorporate the local Bi resonant p-like states with freedom of spin, including spin–orbital coupling [16]. According to the methodology introduced in [16, 27, 30, 31], the 16-band Hamiltonian for InN$_x$Bi$_y$Sb$_{1-x-y}$ can be written as

$$H_{16 \times 16} = \begin{pmatrix}
E_c & 0 & E_c & 0 & P + Q \\
0 & \frac{1}{\sqrt{3}} P_x & 0 & P - Q \\
\frac{1}{\sqrt{3}} P_x & 0 & \frac{1}{\sqrt{3}} P_y & S^* - P - Q \\
0 & \frac{1}{\sqrt{3}} P_y & -\frac{1}{\sqrt{3}} P_x & D - \sqrt{2} S \\
-\frac{1}{\sqrt{3}} P_x & \frac{1}{\sqrt{3}} P_y & -\sqrt{2} R^* & \frac{s}{\sqrt{2}} D - P - \Delta
\end{pmatrix},$$  

\(1\)

where $H_{8 \times 8}$ is the 8-band $k \cdot p$ Hamiltonian of host material given by equation (2) [32], $H_{2 \times 2}$ is the s-like localized N impurity Hamiltonian [22] and $H_{6 \times 6}$ is the Hamiltonian for the p-like localized Bi impurity [27]. The $H_{2 \times 2}$ and $H_{6 \times 6}$ account for the interaction between N and Bi impurity resonate states with the host material states [20, 27]. In the aforementioned Hamiltonian, the effect of the two kinds impurities of N and Bi, namely BAC and VBAC, are extracted from the many-impurity Anderson model [20, 27].

The 8-band Hamiltonian $H_{8 \times 8}$ in equation (1) is given by

$$H_{8 \times 8} = \begin{pmatrix}
E_c & 0 & E_c & 0 & P + Q \\
0 & \frac{1}{\sqrt{3}} P_x & 0 & P - Q \\
\frac{1}{\sqrt{3}} P_x & 0 & \frac{1}{\sqrt{3}} P_y & S^* - P - Q \\
0 & \frac{1}{\sqrt{3}} P_y & -\frac{1}{\sqrt{3}} P_x & D - \sqrt{2} S \\
-\frac{1}{\sqrt{3}} P_x & \frac{1}{\sqrt{3}} P_y & -\sqrt{2} R^* & \frac{s}{\sqrt{2}} D - P - \Delta
\end{pmatrix}. $$  

\(2\)

Detailed expressions of the terms used in $H_{8 \times 8}$ Hamiltonian are given in our previous work [21, 32]. It contains both kinetic terms $H_k$ and strain terms $H_s$.

The strain tensor can be calculated as follows:

$$\epsilon_{xx} = \epsilon_{yy} = \epsilon_{yy} = \frac{a(\text{InSb}) - a(\text{InN}_x\text{Bi}_y\text{Sb}_{1-x-y})}{a(\text{InN}_x\text{Bi}_y\text{Sb}_{1-x-y})},$$  

\(3\)

$$\epsilon_{zz} = -\frac{2C_{12}}{C_{11}}\epsilon_{xx},$$  

\(4\)

where $a(\text{InN}_x\text{Bi}_y\text{Sb}_{1-x-y}) = xa(\text{InN}) + ya(\text{InBi}) + (1 - x - y)a(\text{InSb})$. $C_{11}$ and $C_{12}$ are the elastic stiffness constant.

$H_{2 \times 2}$ is the s-like localized N impurity Hamiltonian and has the form

$$H_{2 \times 2} = \begin{pmatrix}
E_N & 0 \\
0 & E_N
\end{pmatrix},$$  

\(5\)

where $E_N$ is the energy level of the s-like localized N impurity state. Similar to N, $H_{6 \times 6}$ is the Hamiltonian for the p-like localized Bi impurity, and is given by

$$H_{6 \times 6} = \begin{pmatrix}
E_{Bi} & 0 & 0 & 0 & 0 & 0 \\
0 & E_{Bi} & 0 & 0 & 0 & 0 \\
0 & 0 & E_{Bi} & 0 & 0 & 0 \\
0 & 0 & 0 & E_{Bi,so} & 0 & 0 \\
0 & 0 & 0 & 0 & E_{Bi,so} & 0
\end{pmatrix},$$  

\(6\)

where $E_{Bi}$ and $E_{Bi,so}$ are the energy levels of p-like localized Bi impurity state.

The $H_{8 \times 2}$ and $H_{8 \times 8}$ Hamiltonian accounts for the interaction that the host material state has with N and Bi impurities respectively. They are given by equations (7) and (8) respectively.

$$H_{8 \times 2} = \mathbf{V}_N \begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}^\top,$$  

\(7\)
where $V_N$ and $V_{Bi}$ are the coupling coefficients in the BAC model for N and VBAC model for Bi, respectively. All material parameters related to InSb used in this work can be found in table 1, while other parameters corresponding to N and Bi impurities can be found in table 2.

Since here the QW nanostructure is confined along [001] direction, we use plane waves to expand the wave functions. The number of plane waves used is 15.

### Table 1. Parameters of InSb used in our calculation.

| Parameter (unit) | Value |
|------------------|-------|
| $a$ (nm)         | 0.6479|
| $E_p$ (eV)       | 21.2  |
| $E_g$ (eV)       | 0.237 |
| $\gamma_1$      | 37.10 |
| $\gamma_2$      | 16.50 |
| $\gamma_3$      | 17.70 |
| $\Delta_{10}$ (eV) | 0.810 |
| $m$             | 0.014 |
| $a_1$ (eV)      | -6.17 |
| $a_2$ (eV)      | 0.36  |
| $b$              | -2.1  |

* Reference [33].

### Table 2. Parameters of BAC and VBAC used in calculation.

| Parameter (unit) | Value |
|------------------|-------|
| $a$ (InN) (nm)   | 0.498 |
| $a$ (InBi) (eV)  | 0.6626|
| $V_N$ (eV)       | 3.0   |
| $V_{Bi}$ (eV)    | 1.35  |
| $E_N$ (eV)       | 0.65  |
| $E_{Bi}$ (eV)    | -1.20 |
| $E_{Bi,S}$ (eV)  | -2.50 |

* Reference [33].

| Parameter (unit) | Value |
|------------------|-------|
| $a$ (InN) (nm)   | 0.498 |
| $a$ (InBi) (eV)  | 0.6626|
| $V_N$ (eV)       | 3.0   |
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| $E_{Bi}$ (eV)    | -1.20 |
| $E_{Bi,S}$ (eV)  | -2.50 |

* Reference [33].

**2.2. The method of deriving effective Hamiltonian within k · p theory**

In order to investigate the topological transitions in edge states of TIs, we need to construct an effective Hamiltonian like the one introduced by Bernevig et al [5]. The projection of the conventional Hamiltonian from the $k \cdot p$ theory given by equation (1) into the low energy subspace can be done in two steps [28]. First, we divide the Hamiltonian into two parts:

\[
H = H \left( \begin{array}{cc}
0 & -i \frac{\partial}{\partial z} \\
0 & 0
\end{array} \right) + H' \left( \begin{array}{cc}
k_x & k_y \\
-k_y & -i \frac{\partial}{\partial z}
\end{array} \right),
\]

where $H \left( \begin{array}{cc}
0 & -i \frac{\partial}{\partial z} \\
0 & 0
\end{array} \right)$ is the non-perturbative Hamiltonian and $H' \left( \begin{array}{cc}
k_x & k_y \\
-k_y & -i \frac{\partial}{\partial z}
\end{array} \right)$ is the perturbative Hamiltonian. After numerically diagonalizing $H \left( \begin{array}{cc}
0 & -i \frac{\partial}{\partial z} \\
0 & 0
\end{array} \right)$, we obtain the eigenenergies $E_m$ and eigenstates $\psi_m$ where $m$ is the band index. In order to perform the degenerate perturbation calculation, we need to cast the eigenstates of $H \left( \begin{array}{cc}
0 & -i \frac{\partial}{\partial z} \\
0 & 0
\end{array} \right)$ into two classes. The first one, denoted as A class, includes the low energy subspace that we are interested in. The second class, denoted as B class, includes the states that need to be taken into consideration in the subsequent perturbative iteration.
Now, we calculate the effective Hamiltonian according to Lowding perturbation method, given as

\[
H_{eff} = \sum_{m,m'} \left( H_m^{m'} + \frac{1}{2} \sum_{l} H_{ml}^{m'} \left( \frac{1}{E_m - E_l} + \frac{1}{E_{m'} - E_l} \right) \right),
\]

where \( m, m' \in A \) class and \( l \in B \) class. Hence this calls for an appropriate choice of \( A \) class and \( B \) class to construct the effective Hamiltonian which can accurately describe the \( \text{InN Bi Sb}_{1-x-y} / \text{InSb} \) QW bandstructure.

2.3. Method of calculating two-terminal conductance

Based on the effective Hamiltonian, we can calculate the two-terminal conductance of a finite rectangular sample to confirm the existence of topologically protected edge states. At absolute zero temperature, the two-terminal conductance can be expressed by Green’s function as

\[
G = \frac{e^2}{h} \text{Tr} \left[ \Gamma_3 G T_D G^* \right],
\]

where \( G^{R/A} \) is the retarded/advanced Green’s function, and \( \Gamma_{S(D)} = i \sum_{S(D)} - \sum_{S(D)}^{\uparrow/\downarrow} \) with \( \sum_{S(D)}^{\uparrow/\downarrow} \) being the retarded/advanced self-energies due to the source (drain) lead, respectively.

3. Results and discussion

3.1. The phenomenon of band inversion in \( \text{InN Bi Sb}_{1-x-y} / \text{InSb} \) QWs

We have studied \( \text{InN Bi Sb}_{1-x-y} / \text{InSb} \) QWs of varying well thickness and barrier thickness having varying compositions of N and Bi. It was found that topological phase transition can be realized in \( \text{InN Bi Sb}_{1-x-y} \) by suitably increasing the width of the QW. We have considered \( \text{InN Bi Sb}_{1-x-y} \) of well widths 7, 7.7 and 8.2 nm and fixed InSb barrier of width 7.0 nm. The well region had concentrations of N and Bi set to 2.4% and 3.2% respectively, leading to about 0.48% tensile strain. Figures 1(a)–(c) show the electronic bandstructures of these

8 Konig et al.[6] experimentally demonstrated TIs for the first time in HgTe QWs. They found that QWs below a critical thickness had ‘normal’ electronic structure, while those above the critical thickness had an inverted electronic structure. The former showed zero edge state conductance, while the latter exhibited an edge channel transport conductance as expected in a QSH insulator, which was independent of the QW thickness, indicative of the fact that they were edge-states driven.
three cases around the Γ-point demonstrating band-inversion with increasing QW widths. For the narrowest QW of the three (7 nm), the first CB subband (CB1) is at a higher energy than the first VB subband (VB1) as shown in figure 1(a). When the well-width is increased, the CB1 and VB1 tend to approach each other. We found that for a critical well-width of 7.7 nm, gapless state can be achieved where the CB1 and VB1 energies coincide, as shown in figure 1(b) (see footnote 7). However, for well-width larger than the critical width, the CB1 and VB1 states crossover and band-inversion is achieved. For instance, QW of 8.2 nm well-width has an inverted bandstructure as shown in figure 1(c).

Now, we compute the energy bandgaps for InN, Bi, Sb1-x-y/InSb QWs having varying well-width (6–10 nm) and barrier width (6–12 nm). Figure 1(d) shows the bandgap as a function of the width and barrier of the QW. This can serve as a phase diagram for the topological phase transitions, with the positive bandgap corresponding to the trivial phase and negative bandgap corresponding to the non-trivial phase, respectively.

### 3.2. The effective Hamiltonian of InN, Bi, Sb1-x-y/InSb QWs

The band-inversion characteristic of InN, Bi, Sb1-x-y/InSb QWs studied in figure 1 is a necessary but not sufficient condition to establish the existence of QSH effect and topologically protected surface states. But, in order to confirm that the phase exhibiting band-inversion is indeed a topological phase, we will demonstrate the existence of edge states from a quasi-one-dimensional ribbon geometry. To investigate the edge states, we have constructed an effective Hamiltonian according to the theoretical description of equation (10) given in section 2. Our 6-band effective Hamiltonian can be expressed as

$$H^{\text{eff}} = \begin{pmatrix} H(k) & 0 \\ 0 & H^*(\mathbf{-k}) \end{pmatrix}$$  (12)

where $H(k) = \varepsilon(k) I_{3 \times 3} + \mathbf{h}(k)$.

$$\varepsilon(k) = C - Dk^2_{\parallel},$$  (13)

$$\mathbf{h}(k) = \begin{bmatrix} M - Bk^2_{\parallel} & A_2k_+ & A_4k_+ \\ A_2k_+ & -(M - Bk^2_{\parallel}) & Nk^2 \\ A_4k_+ & Nk^2 & (E - Fk^2_{\parallel}) \end{bmatrix},$$  (14)

where $k_{\parallel}$ denotes the in-plane momentum, and $k_{\perp} = k_x \pm i k_y$. The $A_1, A_2, B, C, D, E, F$ and $N$ are expansion parameters that depend on the heterostructure. $M$ is the Dirac mass parameter. The new parameters $E, F$ and $N$ account for the additional VB2 subband in our calculation. These parameters were calculated to be:

$A_1 = -0.4395$ eV nm, $A_2 = -0.2911$ eV nm$^2$, $B = -0.5841$ eV nm$^2$, $C = 0.0347$ eV, $D = -0.4116$ eV nm$^2$, $E = 0.0145$ eV, $F = 0.5114$ eV nm$^2$, $N = 0.1070$ eV nm$^2$, $M = -0.0031$ eV. The Dirac mass parameter $M$ can be continuously tuned from a positive value $M > 0$ for thin QWs with thickness less than the critical thickness (7.7 nm in our case), to a negative value $M < 0$ for thick QWs with thickness less than the critical thickness. For our InN, Bi, Sb1-x-y/InSb QW case of 8.2 nm, we have $M < 0$, which is consistent with that of the CdTe/HgTe QW TI [5, 6].

Unlike the 4-band model of HgTe/CdTe QW case [5], ours is a 6-band model. There are two main reasons for this difference. Firstly, the states most involved in the electronic structure determination are the first conduction subband (CB1) and first valence subband (VB1). The major components contributing to them are light-hole (LH) for CB1 and electron (E) for VB1, as shown in figure 2. But for the HgTe/CdTe QW case, the major components of CB1 and VB1 were heavy-hole (HH) and E, respectively. In our case, it is the tensile strain introduced by impurities that push the LH band higher than the HH band. Secondly, the gap between the VB1 subband and VB2 subband is too small, which leads to strong coupling between the VB1 and VB2 states. Therefore, the projected low energy subspace, A class, needs to include CB1, VB1 and VB2 with the spin degeneracy leading to a 6-band effective Hamiltonian. Another noteworthy point is that the $N$-related terms $Nk_+^2$ in equation (12), takes into account the coupling between HH and E bands.

Now, using our effective 6-band Hamiltonian we will study the QW case of figure 1(c), which demonstrated band-inversion and had a well with 2.4% N and 3.2% Bi impurity doping, a well-width of 8.2 nm and barrier width of 7.0 nm. Figure 3(a) shows the bandstructure of this QW case calculated from the effective Hamiltonian of equation (12) (shown in color lines), which is in good agreement with the bandstructure calculated by full 16-band $k \cdot p$ envelope functions of equation (1) (shown in black lines) near the Fermi energy level. This verifies the validity of our effective Hamiltonian of equation (12).

### 3.3. Edge states and spin-momentum locking phenomenon

Using our newly derived effective Hamiltonian, we have calculated the band structure of a ribbon geometry, as shown in figure 3(b). The red curves show topological edge states which connect the CB and VB. For this ribbon structure, figure 3(c) illustrates that the associated wavefunctions at the ribbon edges for $k_{\parallel} = -0.1, 0.0$ and 0.1
Notice that for $k_0 = -0.1$ and $0.1$ nm$^{-1}$, the wavefunctions are localized at the edges and are spin-momentum locked. This is a typical QSH effect phenomenon demonstrated by 2D TIs [5]. This is the first proof that confirms the TI properties.
Another important term RSS\(^9\) is associated with the splitting of CB or VB when the system is subjected to an external electric field. The RSS of our QW system of figure 1(c) is shown in figure 3(d), where the external electric-field is \(F = 0.5\) mV nm\(^{-1}\). The nonlinear RSS behavior agrees well with the previous results \([22]\). The magnitude of RSS was found to be in the order of 1–2 meV. Such remarkable Rashba spin–orbit coupling offers possibilities of generation, manipulation and detection of spin currents \([36, 37]\).

3.4. The transport properties of edge states

Furthermore, the transport properties of a two-terminal rectangular superlattice sample of dimensions \(L \times N\) are investigated. The two-terminal conductance, \(G\) of a finite sample as a function of Fermi energy is shown in figure 4. Even when the Fermi energy lies in the bandgap window, the conductance, \(G\) is not zero, but has a finite value (here it is \(2e^2/h\)). It exhibits an edge channel transport conductance as expected in a QSH insulator, which is independent of the QW thickness, indicative of the fact that they are edge-states driven. The second proof in the view of the transport properties demonstrates the edge state of TI.

3.5. The effect of magnetic field

The third proof to confirm the TI properties comes from the magnetic field effects consideration. Now we shall investigate the influence of a perpendicular magnetic field \(\mathbf{B} = B\hat{z}\) (without the loss of generality, we assume \(B > 0\)). When the 2D electron gas is subjected to a perpendicular magnetic field, the wavevector get modified as \(\mathbf{k} = -i\nabla + e\mathbf{A},\) where \(\mathbf{A}\) is the vector potential such that \(\mathbf{B} = \nabla \times \mathbf{A}.\) The Zeeman energy induced by the magnetic field here is ignored. Here, we choose the Landau gauge \(A = (-By, 0, 0).\) The Laudau levels (LLs) can be found by defining the two ladder operators \(a = -\left(\frac{\partial}{\partial y} + l_B\partial_x - l_Bk_x\right)/\sqrt{2},\) and
\[
a^\dagger = -\left(\frac{\partial}{\partial y} - l_B\partial_x - l_Bk_x\right)/\sqrt{2},
\]
where the magnetic length \(l_B = \sqrt{\hbar/eB}.\) Now, we assume the following trial solution
\[
\psi_n(x, y) = \frac{1}{\sqrt{L_x}} e^{ik_x x} \begin{pmatrix} C_{n\uparrow} [n] \\ C_{n\downarrow} [n + 1] \\ C_{n\uparrow} [n - 1] \\ C_{n\downarrow} [n] \\ C_{n\uparrow} [n - 1] \\ C_{n\downarrow} [n + 1] \end{pmatrix},
\]
\[n \geq 1,\]  
\[
(15a)
\]

\(^9\) RSS stands for Rashba spin-splitting, which is a momentum-dependent splitting of spin bands in semiconductor heterostructures.
where \( n = 0 \),

\[
\psi_n(x, y) = \frac{1}{\sqrt{L_x}} e^{\frac{ik}{a}y} \begin{pmatrix} C_{n\uparrow} \left( 0 \right) \\ C_{n\downarrow} \left( 1 \right) \\ 0 \\ C_{n\uparrow} \left( 0 \right) \\ 0 \\ C_{n\downarrow} \left( 1 \right) \end{pmatrix}
\]

As Buhmann et al. \[38\] have stated, that there will be a crossing point between zero-mode LLs for topological phase while there will be no crossing point for normal phase; this can be used to verify the topological phase transition. Figure 5 gives the LLs structure. The crossing point between the two LLs labeled by red curves indicates the existence of topological band inversion at zero magnetic field \[38\] as the case of the CdTe/HgTe QW \[6\].

3.6. Topological transition phase with different concentration of the two impurities

Having studied the band inversion in InN\(_x\)Bi\(_y\)Sb\(_{1-x-y}\) QWs of fixed N and Bi composition, we would like to study the effect of the impurity doping concentration on its properties. The possibility of the use of InN\(_x\)Bi\(_y\)Sb\(_{1-x-y}\) QWs as TIs opens up avenues for designing TIs with effective bandgap and strain tuning by varying the doping concentrations of N and Bi. For the same, we have studied a range of QWs with fixed well-width of 7.0 nm and barrier width of 7.0 nm and varying N composition (0%-4%) and varying Bi composition (0%-8%). Figure 6 shows the topological phase diagram for the topological phase transitions showing the variation in bandgap as a function of N and Bi concentration. The whole region is divided into two different phases: the positive bandgap corresponds to the trivial phase and negative bandgap corresponds to the non-trivial phase, respectively. A prominent feature is that the boundary separating the positive and negative bandgap regions is a broken line. This is different from figure 1(d) in which the boundary is a straight line. We explain the reason here. Changing the well-width and barrier-width keeps the strain invariant (equations (3) and (4)), while different concentrations of N and Bi impurities leads to varying degrees of tensile or compressive strain. The type of the strain directly determines the highest valence subbands (VB1). Tensile strain corresponds to \( \uparrow \downarrow \)\(BH\), while compressive strain corresponds to [HH \[\uparrow \downarrow \]] subbands as the highest valence subbands. Therefore, the kind of the phase boundary in figure 6 corresponds to the differences arising from these two strain cases.

4. Summary and conclusion

We have proposed a practical scheme to realize QSH effect and topological phase transitions in InN\(_x\)Bi\(_y\)Sb\(_{1-x-y}\)/InSb QW. The well-width, barrier-width and concentrations of N and Bi impurity doping can be used to effectively attain band-inversion as we have comprehensively demonstrated. The coupling between the impurity resonant states is critical and has a profound effect on the narrowing down of the bandgap until band-inversion occurs.

In summary, we have confirmed the (i) band-inversion in InN\(_x\)Bi\(_y\)Sb\(_{1-x-y}\) QWs above a certain critical thickness (figures 1 and 2), (ii) topologically protected edge-states using bandstructure analysis (figure 3(b)), (iii) edge-localized distribution of the wavefunctions and edge-state spin-momentum locking phenomenon (figure 3(c)), (iv) presence of non-zero Hall conductance in spite of the Fermi energy lying in the bandgap
In conclusion, with all of the aforementioned characteristics in view, we are in a position to confirm the existence of QSH effect and topological phase transitions in InN\textsubscript{\textit{x}}Bi\textsubscript{\textit{1-x}}Sb\textsubscript{\textit{1-y}}/InSb QWs as a proof-of-concept.

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Figure 6. A phase diagram for the topological phase transitions showing the variation in bandgap as a function of \( N \) and Bi concentration. Similar to figure 1(d), the region is divided into two different phases: the positive bandgap corresponds to the trivial phase and negative bandgap corresponds to the non-trivial phase, respectively. Here, the well-width and barrier-width is fixed at 8.2 nm and 7.0 nm, respectively. The magnitude of negative band gap can exceed the 60 meV mark. This is essential for practical implementation of TIs.
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