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Three-dimensional Topological Insulator Tunnel Diodes

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Topological insulators open many avenues for designing future electronic devices. Using the Bardeen transfer Hamiltonian method, we calculate the current density of electron tunneling between two slabs of Bi_2Se_3 . 3D TI tunnel diode current-voltage characteristics are calculated for different doping concentrations, tunnel barrier height and thickness, and 3D TI bandgap. The difference in the Fermi levels of the slabs determines the peak and valley voltages. The tunnel barrier width and height affect the magnitude of the current without affecting the shape of the current-voltage characteristics. The bandgap of the 3D TI determines the magnitude of the tunnel current, albeit at a lesser rate than the tunnel barrier potential, thus the device characteristics are robust under changing TI material. The high peak-to-valley ratio of 3D TI tunnel diodes, the controllability of the valley current location, and the simple construction provide advantages over other NDR devices.

I. INTRODUCTION

Topological insulators (TI) are a class of material with spin-momentum locked helical surface or edge states. Topological insulators are classified as either two-dimensional (2D) or three-dimensional (3D). A 2D TI has an insulating 2D bulk and a conducting edge, while a 3D TI has an insulating bulk and conducting surface. 3D TIs are arguably more promising for short-term device applications than 2D TIs because well-known materials like Bi_2Se_3 are 3D TIs while 2D TIs rely on more exotic materials [28] like stanene [7, 39] and bismuthene [33].

In Bi_2Se_3 and related topological insulators, spin-orbit interactions lead to the quantum spin Hall effect. The quantum spin Hall effect is associated with an insulating bulk and conducting gapless edge states. Specifically for 3D TIs like Bi_2Se_3 , if the energy of spin-orbit coupling is larger than some critical value, the order between two energy levels nearest the Fermi energy is reversed. Because these two energy levels have an opposite parity, this drives the system into a topological insulator phase [9].

Surface states of 3D TIs have the interesting property that they have a Dirac dispersion and that their spin and momentum is locked [25]. Previous device proposals have exploited the spin-momentum locking to convert charge to spin [32]. Here we will take a different approach and exploit the spin-momentum locking of 3D TI surface states to block tunneling current and realize an NDR device [29].

Recent advances in the field of topological insulators [8] have opened a plethora of opportunities for their use in both charge-based [25, 28] and spin-based devices [13, 16]. TIs have been proposed for many exotic applications including quantum computation [10], lasing [1], and skyrmion-based devices [34]. Some recent proposed applications are electrochemical energy storage [36] and

mode-locked lasers [37]. Electric-field control of the surface state spin-polarization opens a plethora of opportunities in building spin-based devices using Bi_2Se_3 including, superconductivity [6], photodetectors [24], and terahertz frequency generation [22].

Negative-differential resistance (NDR) devices are a class of electronic devices with non-linear current-voltage characteristics. Specifically, they have regions in which their current decreases with increasing voltage. Due to their unusual response to applied voltage, they are used in many applications such as fast memories, high-frequency devices, frequency-multipliers, and fast switching devices [35].

Unfortunately, present day NDR devices are less controllable in terms of the location of the minima and come with a fixed peak-to-valley ratio [27], which is the ratio of the maximum current to that of the current at the minimum. Although some devices based on nanoscale molecular junctions [4], and graphene nanoribbons [19] have been proposed to remedy the relatively little control possessed in many current the NDR devices, the difficulty in fabricating such devices presents a roadblock for their practical application [15, 21]. The difficulty in fabricating 2D NDR devices has been noted in both graphene nanoribbons [15], and graphene quantum dots [23]. The development of a 3D TI NDR device could potentially solve many of these issues.

In this work, we investigate a two-terminal NDR device using two 3D TI slabs separated by a tunnel barrier. First, we model the electronic structure of 3D TIs and present the theoretical formulation for calculating the tunneling current. We then show the NDR characteristics of the proposed device and discuss various control parameters such as device geometry and TI material selection which can be tuned to control the characteristics of the device. We show that the presented device

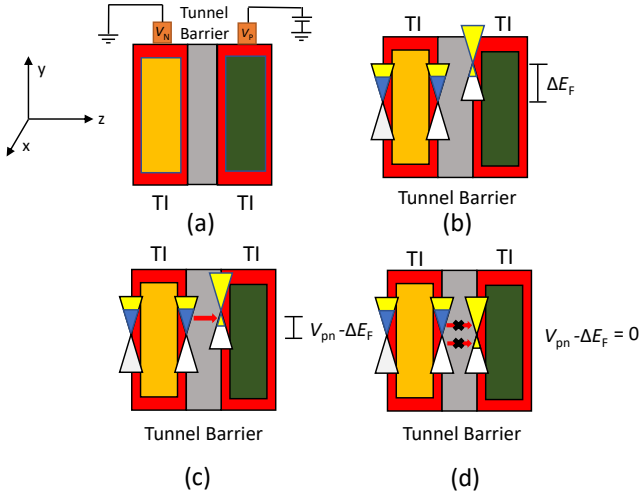


FIG. 1: (a) Device schematic for our proposed TI tunnel diode NDR device. The top slab (green) is p -doped and connected to bias while the bottom slab (yellow) is n -doped and grounded. The p -doped and n -doped slabs have thickness $t_p = t_n = 10$ nm. The tunnel barrier's default thickness is $t = 1.0$ nm. (b) Relative position of TI slab Dirac cones due to ΔE_F at zero bias. (c) Relative position of the TI slab Dirac cones at bias V_{pn} less than ΔE_F where finite tunneling current is present between the TI slabs. (d) Relative position of the TI slab Dirac cones at bias V_{pn} equal to ΔE_F where spin polarization prevents tunneling between the TI slabs.

provides a very high peak-to-valley ratio along with an efficient control over the position of the valley current, the location of the minimum of the current in the NDR region. Finally we discuss the results and their implications and conclude.

II. DEVICE STRUCTURE AND THEORETICAL MODEL

II.1. Device Structure

Figure 1(a) shows the schematic of the Bi_2Se_3 device under investigation. The device comprises of two TIs separated by a tunnel barrier. The two slabs of Bi_2Se_3 are assumed to have a different Fermi level as determined by their doping [3, 30]. We choose Bi_2Se_3 because it is the most studied 3D TI, but our findings apply to any material with a spin-polarized Dirac cone and $\mathbb{Z}_2$ topological order. The spin-polarized conducting surface states are illustrated by the surfaces of the two slabs. The top and bottom slabs are given different colors in our schematic to reference the difference in the Fermi levels (ΔE_F) of the two slabs shown in Fig. 1(b).

The top slab, which is p -doped, is connected to a voltage source to set the bias V_{pn} and the bottom slab, which is n -doped, is grounded. The total device thickness in our

simulations is taken to be 21 nm with a slab size of 10 nm for the p -doped and the n -doped slabs, and a tunnel barrier thickness of 1 nm. Our device's layered nature allows the thickness of the tunnel barrier to be controlled. Translational symmetry is assumed in the transverse x and y directions.

II.2. Device Operation

Figure 1 (b-d) illustrate the position of the Dirac cones of the surface states of both the slabs at different applied bias (V_{pn}). Fig. 1(b), shows the Dirac cones when no bias is applied ($V_{pn}=0$). In Fig. 1(c), the Dirac cone of the top slab shifts down due to an applied bias $0 < V_{pn} < \Delta E_F$. With an applied bias, a finite tunneling current flows between the slabs as indicated by the red arrow. The tunneling occurs between the surface states of the n -doped and p -doped slabs. Fig. 1(d), shows the case when the applied bias equals the Fermi level difference ($V_{pn} = \Delta E_F$), the Dirac cones of the surface states now match perfectly. However, the surface states have opposite spin-momentum locking which will make the tunneling current vanish. Momentum and energy can be conserved but spin cannot be conserved because of the opposite spin-polarization of both surface states. A more detailed examination of the effects of spin-polarized surface states on the tunneling current is presented in III.1.

In Sec. III.II we will show how this device responds to changes to key device parameters. The first of these properties of the tunnel barrier, specifically its width and potential or height, both of which can be simply controlled. We will also show how the effects on the Fermi level through doping affect device performance. Finally, we will examine the effects of changing the TI material which can also model how chemical or mechanical strain on Bi_2Se_3 might impact device behavior.

II.3. Electronic Structure of Slabs

We model the TIs and the tunnel barriers using a $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian to describe the TI device performance. We use the Bi_2Se_3 Hamiltonian from Ref. [38].

$$\mathcal{H}(\mathbf{k}) = \epsilon_0(\mathbf{k})\mathcal{I} + \begin{pmatrix} \mathcal{M}(\mathbf{k}) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}(\mathbf{k}) & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}(\mathbf{k}) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}(\mathbf{k}) \end{pmatrix} \quad (1)$$

where $k_{\pm} = k_x \pm ik_y$, $\epsilon_0(\mathbf{k}) = C + D_1 k_z^2 + D_2(k_x^2 + k_y^2)$, $\mathcal{I}$ is a 4×4 identity matrix, and $\mathcal{M}(\mathbf{k}) = M - B_1 k_z^2 - B_2(k_x^2 + k_y^2)$. The directions x, y are defined as being in-plane with the TI surface. The z direction is defined as being the out-of-plane direction. k_x, k_y , and k_z are the wave-vector components in the x, y , and z directions. This Hamiltonian keeps terms up to quadratic order in $\mathbf{k}$.

The biases under study for our device range from 0.0 eV to 0.2 eV. This range of energies only requires that we consider the low energy behavior of our TI Hamiltonian. This low energy Hamiltonian accurately models the ground and first excited energy eigenstates of our TI device [17], which, is sufficient to accurately model the J-V curves of our device as topological nature of Bi_2Se_3 is determined by the physics near the Γ -point. In Section VI.2 we show that considering only the ground and first excited state energy eigenstates is sufficient to accurately model device behavior. The eigenvalues of this Hamiltonian display rotational symmetry in the transverse directions k_x and k_y in this low-energy approximation.

The parameters B_1 , B_2 , C , D_1 , D_2 , and M are presented in Table I in Section VI.I and were previously determined for Bi_2Se_3 in Ref. [38] by fitting to the bulk Bi_2Se_3 band structure obtained from *ab initio* DFT calculations. These parameters give us the slab Hamiltonian $\mathcal{H}_{\text{TI},p}$ and $\mathcal{H}_{\text{TI},n}$.

We use vacuum as the interface tunnel barrier as Bi_2Se_3 is a Van der Waals material. To model the Hamiltonian of this tunnel barrier, $\mathcal{H}_T$, we set parameters to that of a free electron with a 1 eV on-site potential [25] to mimic a tunnel barrier with a 1 eV barrier. The parameters $D_1 = D_2 = 3.8 \text{ eV } \text{\AA}^2 = \hbar^2/(2m_e)$, where $\hbar$ is the reduced Planck constant, are chosen to give the electron the free electron mass in the tunnel barrier.

Any material which has a barrier mismatch could, in principle, be used as a tunnel barrier for this device. Since the topological insulator has surface states and a significant amount of charge on the surface, we assume the entire voltage is dropped over the tunnel barrier. Gapped van der Waals materials like transition-metal dichalcogenides (TMDs) are ideal because of the lack of dangling bonds, making defect formation less likely.

To apply a Fermi shift of ΔE_F , we add a term ΔE_F to the diagonal elements of the Hamiltonian in Eq. (1). We apply a bias by subtracting V_{pn} from ΔE_F and treating this as the new effective Fermi shift for $\mathcal{H}_{\text{TI},p}$.

In Fig. 2, we show the band structure of a TI slab. The left side of Fig. 2 represents the bottom, n -doped, slab without any Fermi level shift, while the right side represents the top, p -doped, slab with a Fermi level shift of 0.10 eV at zero applied bias. The p -doped and n -doped Fermi levels are represented by dotted lines. The opposite spin polarizations are represented by red and green shading. It can be observed that doping has created a difference between the p -doped and n -doped Fermi levels. We obtain the topological surface states by solving our model Hamiltonian with an open boundary condition [18]. To compute the wave functions in the out-of-plane direction, z , we convert k_z to $i \frac{d}{dz}$, and discretize the Hamiltonian in Eq. (1) using finite differences as detailed in Sec. VI.1. The spin-polarized surface states of the top and bottom slab have different energies because of the 0.1 eV relative Fermi level difference.

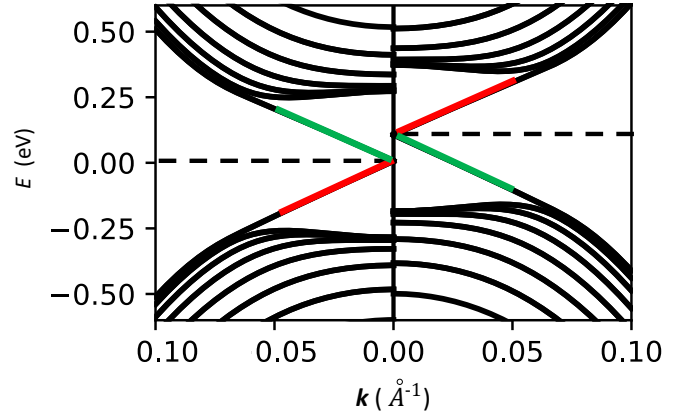


FIG. 2: Band structure of a TI slab of 10 nm thickness plotted in transverse direction $k = \sqrt{k_x^2 + k_y^2}$. The left hand side corresponds to the n -doped TI slab of Fig. 1(b) and has no Fermi level shift, while the right hand side corresponds to the p -doped TI slab of Fig. 1(b) and has a Fermi level shift ΔE_F of 0.1 eV. The dotted lines represent the effective Fermi level of the p -doped and n -doped slabs with this Fermi level shift. The red and green shading represent the spin-polarized region of the surface bands. Red coloration represents one spin polarization, while the green represents the opposite polarization.

II.4. Tunneling Current

We use the Bardeen transfer Hamiltonian method [2] to calculate the tunneling current between the TI slabs. The Bardeen transfer Hamiltonian follows from time-dependent perturbation theory [26], which treats the Hamiltonian of the intervening barrier as a perturbation. We sum over the intersecting pairs of bands μ_j and η_j with band index j . By integrating over the 1D first Brillouin zone and by requiring energy conservation, the current is determined by the intersection of $E_{p\mu}(k)$ and $E_{n\eta}(k)$. Here, we have expressed the band energies of these bands in terms of k by making the substitution $k_+k_- = k^2$. Summing over pairs of intersecting bands with index μ and η leads to the probability of transition between the p -doped and n -doped slabs

$$P = \frac{2\pi}{\hbar} \sum_j \int \int \frac{dk_x}{2\pi} \frac{dk_y}{2\pi} |M_j|^2 \delta(E_{n\mu_j}(k) - E_{p\eta_j}(k)) \quad (2)$$

where

$$|M_j| = \left| \Psi_{n\mu_j}(\kappa_j) \frac{d\Psi_{p\eta_j}(\kappa_j)}{dz} - \Psi_{p\eta_j}(\kappa_j) \frac{d\Psi_{n\mu_j}(\kappa_j)}{dz} \right| \quad (3)$$

is the transition matrix element corresponding to the transition between the wave functions of bands $E_{p\mu}(k)$ and $E_{n\eta}(k)$ for $k = \sqrt{k_x^2 + k_y^2}$.

Since our Hamiltonian exhibits in-plane rotational symmetry, we convert to a polar coordinate system where

$k_x = k \cos(\theta)$ and $k_y = k \sin(\theta)$. We use $k^2 = k_x^2 + k_y^2$ and $dk_x dk_y = k dk d\theta$ to arrive at:

$$P = \frac{1}{\hbar} \sum_j \int k dk |M_j|^2 \delta(E_{n\mu_j} - E_{p\eta_j}) \quad (4)$$

Since our TI Hamiltonian exhibits rotational symmetry, and thus its eigenvalues can be written as dependent only on k , we can straightforwardly convert the delta function as a function of energy in Eq. (4), to be a function of k . We integrate over the first Brillouin zone and require energy conservation. To integrate over k we change $\delta(E_{p\mu} - E_{n\eta})$ to a function of k using

$$\delta(E_{n\mu} - E_{p\eta}) = \delta(k_{n\mu} - k_{p\eta}) \left| \frac{d((E_{p\mu}(k) - E_{n\eta}(k)))}{dk} \right|^{-1}.$$

Evaluating the integral in Eq. 4:

$$P = \frac{1}{\hbar} \sum_j \kappa_j \left| \frac{d(E_{p\mu_j}(k) - E_{n\eta_j}(k))}{dk} \right|_{k=\kappa_j}^{-1} |M_j|^2 \quad (5)$$

where κ_j is the k value at the intersection point.

To model the current density resulting from this transmission probability, we multiply by the electron charge q and the difference in the Fermi-Dirac distribution functions $f(E_n) - f(E_p)$:

$$J = \frac{q}{\hbar} \sum_j \kappa_j |M_j|^2 \left| \frac{d(E_{p\mu_j}(k) - E_{n\eta_j}(k))}{dk} \right|_{k=\kappa_j}^{-1} (f(E_{p\mu_j}(\kappa_j) - V_{pn}) - f(E_{n\eta_j}(\kappa_j))) \quad (6)$$

where V_p and V_n are the n -doped and p -doped voltages, respectively, whose difference is V_{pn} .

We use 4500 k -points to calculate the band structure of the slabs. We take a step size of $\Delta z = 1 \text{ \AA}$. We model the performance of our TI device at room temperature. We consider the eight energy bands closest to the Fermi level in the calculation of the current as these bands give the largest contribution to tunneling current. Because of the bands considered, we only encounter, at most, one intersection between any two bands. In the case of multiple intersections a summation over a different κ would be required. Calculating additional bands gives additional possibilities for tunneling and thus increases the current, but this increase does not change the shape of the J-V curves and the increase in the magnitude of the current density quickly becomes negligible. A more detailed examination of the change in the current which results from calculating additional bands can be seen in VI.2.

III. RESULTS AND DISCUSSION

III.1. Current Density

Figure 3 shows the calculated current density J as a function of V_{pn} with Fermi level shifts (ΔE_F) of 0.05 eV, 0.10 eV, and 0.15 eV on the p -doped slab. These Fermi

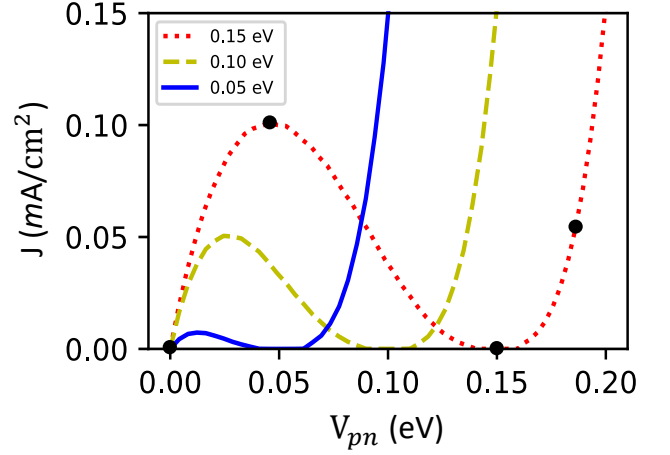


FIG. 3: Current density of our proposed TI NDR device with Fermi level shift $\Delta E_F = 0.05 \text{ eV}$, $\Delta E_F = 0.10 \text{ eV}$, and $\Delta E_F = 0.15 \text{ eV}$. The valley current location on the J-V curve is determined by the Fermi level of the p -doped slab. The black dots represent bias points for which the band structure and wave functions are calculated in Fig. 4

level shifts characterize the how changing the doping of the TI slabs affects device behavior. We observe that the current initially increases linearly with the applied V_{pn} . However, at $V_{pn} \approx \Delta E_F/3$, the current peaks and starts decreasing and goes to almost zero at $V_{pn} = \Delta E_F$, resulting in NDR behavior. Interestingly, we find that unlike conventional NDR devices whose valley current remains finite [27], because of the very small valley current, the peak to valley ratio is very high. For bias $V_{pn} > \Delta E_F$, the current starts to increase again. We also observe from Fig. 3 that the maximum current and the valley bias are both determined by the difference in the Fermi level between the TI slabs.

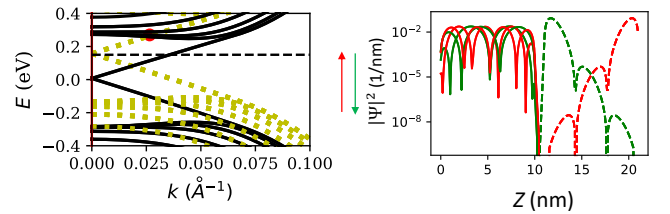


FIG. 4: Band structure of Bi_2Se_3 for applied bias $V_{pn} = 0.0 \text{ eV}$ corresponding to the first dot in Fig. 3. The solid black line represents the n -doped slab and the dotted yellow line represents the p -doped slab. The red dot indicates a chosen intersection for consideration with the wave functions calculated at that intersection point are plotted to the right. Here, we have an intersection between a bulk state and an edge state and no current

To further analyze the device characteristics, we show the band structure and the wave function of the p -doped and the n -doped TI slab at $V_{pn} = 0 \text{ eV}$, 0.05 eV , 0.15 eV , and 0.18 eV in Fig. 4, 5, 6, 7 respectively. We choose

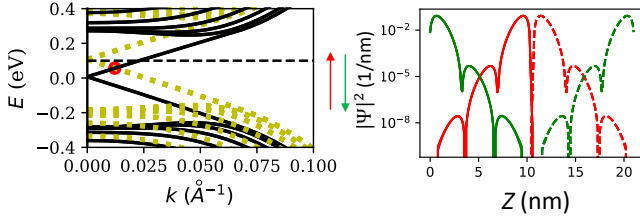


FIG. 5: Band structure of Bi_2Se_3 for applied bias $V_{\text{pn}} = 0.05$ eV corresponding to the second dot in Fig. 3. The solid black line represents the n -doped slab and the dotted yellow line represents the p -doped slab. The red dot indicates a chosen intersection for consideration with the wave functions calculated at that intersection point are plotted to the right. Here, we have two same-spin surface state intersections and finite tunneling current.

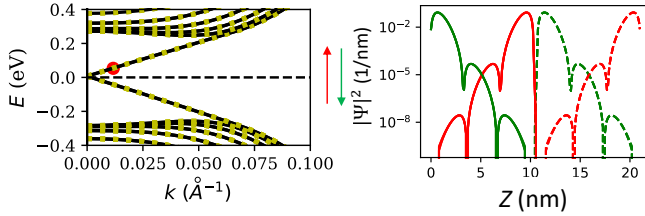


FIG. 6: Band structure of Bi_2Se_3 for applied bias $V_{\text{pn}} = 0.15$ eV corresponding to the third dot in Fig. 3. The solid black line represents the n -doped slab and the dotted yellow line represents the p -doped slab. The red dot indicates a chosen intersection for consideration with the wave functions calculated at that intersection point are plotted to the right. Here, we have two opposite-spin surface state intersections and nearly zero tunneling current.

a $\Delta E_F = 0.15$ eV, which corresponds to the red dotted curve in Fig. 3. The wave functions on the right are calculated at an intersection point between the two bands for each bias point.

Figure 4 shows the band structure and the wave functions at $V_{\text{pn}} = 0$ eV. This corresponds to the first black dot in Fig. 3. Although there are states available for tunneling, the zero bias causes the tunneling current to remain zero (first black dot in Fig. 3).

Figure 5 shows the band structure and the wave functions at a bias $V_{\text{pn}} = 0.05$ eV which corresponds to the second black dot in Fig. 3. We now have two, same-spin surface states intersecting shown by the red dot in Fig. 5 (band structure). We see that the wave functions of the same spin overlap results in a finite tunneling current. We see in Fig. 3 that the tunneling current increases from zero bias up until a bias which is approximately one third of the Fermi level difference between the two slabs.

Figure 6 shows the band structure and the wave functions at a bias $V_{\text{pn}} = 0.15$ eV. This corresponds to the third black dot in Fig. 3. Now, we have two opposite-spin surface states intersecting. Although the wave functions

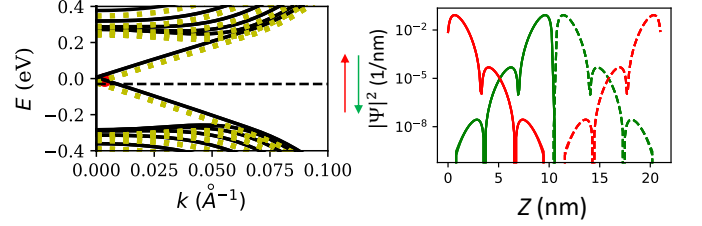


FIG. 7: Band structure of Bi_2Se_3 for applied bias $V_{\text{pn}} = 0.18$ eV corresponding to the fourth dot in Fig. 3. The solid black line represents the n -doped slab and the dotted yellow line represents the p -doped slab. The red dot indicates a chosen intersection for consideration with the wave functions calculated at that intersection point are plotted to the right. Here, we have two same-spin surface states intersections and finite tunneling current.

of the top and the bottom slab have a significant spatial overlap, their opposite spin causes the tunneling current to become very low (as shown in the third black dot in Fig. 3), resulting in a very low valley current for the device.

Figure 7 shows the band structure and the wave functions at a bias $V_{\text{pn}} = 0.18$ eV. This corresponds to the final black dot in Fig. 3. We see that the wave functions of the same spin overlap resulting in a finite tunneling current.

To quantify the overlap, we inspect the transition element for different bias conditions. For a bias of 0.05 eV, the transition element $|M|^2 = 2.32 \times 10^6$ (eV)². At the point where $V_{\text{pn}} = \Delta E_F = 0.15$ eV the transition element is significantly lower at $|M|^2 = 1.10$ (eV)². At $V_{\text{pn}} = 0.18$ eV, significantly larger than ΔE_F , the transition element has once again increased to be on the same order as for 0.05 eV bias at $|M|^2 = 1.76 \times 10^6$ (eV)². The transition element in the case of $V_{\text{pn}} = 0.18$ eV being lesser gives rise to lower current as compared to $V_{\text{pn}} = 0.05$ eV as can be seen in comparing the values of the current at the second and fourth black dots in Fig. 3. Both $V_{\text{pn}} = 0.05$ eV and 0.18 eV have a significantly higher M value than the value at $V_{\text{pn}} = \Delta E_F$.

III.2. Parametric Device Analysis

When studying the NDR tunneling current, there are several parameters of interest. The first of these parameters is the relative Fermi level of the two slabs. The second parameter is the barrier height and barrier thickness. The final parameter is the bandgap of the slabs, the range of energy between the surface states and the first bulk states.

Figure 8(a) shows the current density as a function of applied bias for tunnel barrier thickness $t=1.0$ nm, $t=1.5$ nm, and $t=2.0$ nm. The shape of the current density remains the same, as does the biases at which the peak and valley currents occur. However, as the thickness of

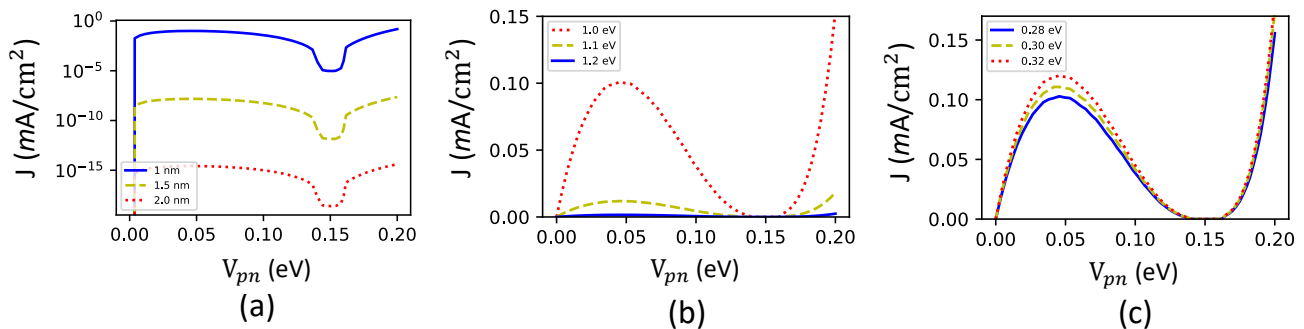


FIG. 8: (a) Current density of our proposed TI NDR device for tunnel barrier thicknesses of $t = 1.0$ nm, 1.5 nm, and 2.0 nm. The magnitude of the current decreases while the shape remains constant as barrier width increases (b)

Current density of the NDR device with tunnel barrier heights of $V_{\text{onsite}} = 1.0$ eV, 1.1 eV and 1.2 eV. The magnitude of the current decreases while the shape remains constant with increasing barrier height. (c) Current density for the NDR device with band gaps $E_g = 0.28$ eV, 0.30 eV, and 0.32 eV. Changing the bandgap has little impact on the current density.

the tunnel barrier between the slabs increases, the magnitude of the current rapidly decreases. This is expected as increasing the gap between the TI slabs decreases the tunneling probability.

Figure 8(b) shows the current density for the tunnel barrier on-site potentials $V_{\text{onsite}} = 1.0$ eV, 1.1 eV, and 1.2 eV. The magnitude of the current density decreases with increasing tunnel barrier on-site potential. The increasing potential increases the tunnel barrier. Since the TIs are unaltered, only the magnitude is affected, not the shape of the J-V curve.

Figure 8(c) shows how the current density changes when the TI bandgap $E_g = 0.28$ eV, 0.30 eV, or 0.32 eV. E_g sets the value of M in the TI Hamiltonian. Changes in the bandgap could be practically realized through chemical or mechanical strain [14], or a different hypothetical 3D TI. The small divergence from the results for Bi_2Se_3 show that another 3D TI will yield J-V characteristics similar to the ones we calculated for Bi_2Se_3 and the small dependence of the J-V on TI bandgap. The peak current increases when the bandgap increases from 0.28 eV to 0.32 eV. The relatively small change suggests that changing the TI of both slabs has little impact on the overall current density as long as the Dirac cone is maintained in the bandgap.

IV. CONCLUSION

We have presented a NDR device based on 3D Bi_2Se_3 slabs sandwiching a tunnel barrier material. The presented device utilizes the spin-momentum locking of the surface states of 3D TIs resulting in a spin-dependent tunneling. We used the Bardeen Transfer Hamiltonian method, we calculated the tunneling current between the two slabs. We have shown that the presented NDR device, unlike conventional NDR devices, can have a valley current almost zero resulting in a very high peak to valley ratio. Recent devices, such as van der Waals nanostruc-

tures and InAs/GaSb Core-Shell Nanowires [5, 12] show peak to valley ratios of 4 [5] and 8.69 [12] respectively. This is significantly lower the peak to valley ratio of our device. While the ideal system tested here presents a very low valley current, impurities in a real device may cause the current in a real device to be higher. Also, if the sample is semimetallic instead of insulating, we may also see a small amount of tunneling between the metallic states. Nevertheless, this device still has lower valley current than other devices. The V_{pn} at which the valley current occurs can be tuned by tuning the Fermi level shift between both slabs. We have seen that the peak of these J-V curves occurs at $V_{\text{pn}} \approx \Delta E_F/3$. Moreover, we have shown that changing the TI material does not have a significant impact on the shape of the J-V curve the device produces. The two-terminal architecture of the presented 3D tunnel diodes makes our proposed device easy to manufacture [3] and conduct experiments on as compared to other NDR devices such as graphene nanoribbons and graphene quantum dots. The proposed device can be fabricated using molecular beam epitaxy [11, 31] [20].

V. ACKNOWLEDGEMENTS

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VI. APPENDIX

VI.1. Calculating Band Structure and Wave Functions for a TI Slab

	Bi ₂ Se ₃	Tunnel barrier
M	0.28 eV	0 eV
A_1	2.2 eV Å	0 eV Å
A_2	4.1 eV Å	0 eV Å
B_1	10 eV Å ²	0 eV Å ²
B_2	56.6 eV Å ²	0 eV Å ²
C	-0.0068 eV	1 eV
D_1	1.3 eV Å ²	3.8 eV Å ²
D_2	19.6 eV Å ²	3.8 eV Å ²

TABLE I: $\mathbf{k} \cdot \mathbf{p}$ parameters for Bi₂Se₃ [38] and the tunnel barrier. These values are used unless noted otherwise.

To calculate the band structure of a TI slab we start with the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian from equation (1). To get a slab band structure as opposed to a bulk band structure, we discretize in the out-of-plane direction by replacing k_z with $-i\frac{d}{dz}$, employing the treatment described by Qi et al.[18]. To find the band structures numerically we use finite differences so that $\frac{df}{dz} \approx \frac{f(z+\Delta z) - f(z-\Delta z)}{2\Delta z}$ and $\frac{d^2f}{dz^2} \approx \frac{f(z+\Delta z) - 2f(z) + f(z-\Delta z)}{(\Delta z)^2}$ where Δz is the step size. In our case, we took a step size of $\Delta z = 1$ Å. This leads to $n_{\text{TI}} = 100$ discrete steps in the TI slab and $n_B = 110$ steps in the tunnel barrier. The systems of the p -doped and n -doped slabs are overlaid, meaning the effective barrier size is equal to the total system size minus 2 times the TI slab size. To solve the Hamiltonian numerically, for both the slab and tunnel barrier Hamiltonians, we take a Kronecker product of the $\mathcal{H}_{\text{TI}}$ and an identity matrix of dimensions of 100×100 for the slab and a Kronecker product of $\mathcal{H}_D$ and identity matrix of dimensions 110×110 for the tunnel barrier. Note that prior to accounting for transitions using the Bardeen Transfer Hamiltonian, when considering the n -slab, the p -slab is modeled using the tunnel barrier Hamiltonian and vice versa.

However, since we are calculating the band structure of the slab with a connected tunnel barrier, we must combine our slab and tunnel barrier Hamiltonians to account for a single system. We define Hamiltonians for each TI slab with a tunnel barrier as shown in Eq. (7) for the p -doped slab and Eq. (8) for the n -doped slab

$$H_p = \begin{pmatrix} H_D & W_{T,D} \\ W_{B,TI} & H_{TI} \end{pmatrix} \quad (7)$$

$$H_n = \begin{pmatrix} H_{TI} & W_{T,TI} \\ W_{B,D} & H_D \end{pmatrix} \quad (8)$$

Here the numerically evaluated Hamiltonians contain the slab and tunnel barrier Hamiltonians as the diagonal elements and connection terms W as the off-diagonal elements.

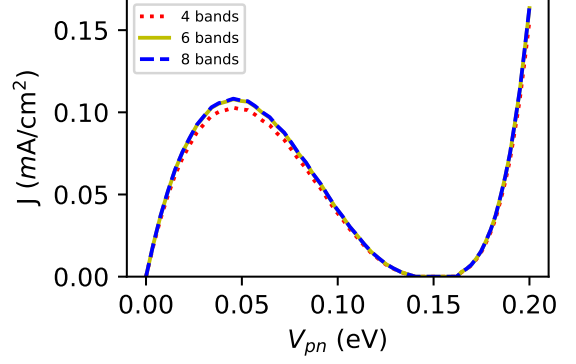


FIG. 9: Current density for a TI slab with increasing number of calculated bands.

The dimensions of the connection terms $4n_{\text{TI}} \times 4n_D$. The connection terms are zero matrices with the exception of 4 elements in the bottom left corner for $W_{T,TI}$ and $W_{T,D}$ and the top left corner for $W_{B,TI}$ and $W_{B,D}$. The exact form of W_T can be seen in Eq. (9) with W_B being the adjoint of W_T .

$$W_T = \frac{-D_1}{(\Delta z)^2} \begin{bmatrix} 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \dots & \dots & \dots & \vdots \\ \vdots & \vdots & \vdots & 0 & 0 & \dots & \vdots \\ \vdots & \vdots & 0 & 1 & 0 & \dots & \vdots \\ \vdots & 0 & 1 & 0 & \vdots & \vdots & \vdots \\ 0 & 1 & 0 & \dots & \ddots & \vdots & \vdots \\ 1 & 0 & \dots & \dots & \dots & \dots & 0 \end{bmatrix} \quad (9)$$

$$W_B = W_T^\dagger \quad (10)$$

VI.2. Change in Current Density with Increasing Calculated bands

In Fig. 9 we can see the current density plotted for 4 bands, 6 bands, and 8 bands calculated at $\Delta E_F = 0.15$ eV. We see that the magnitude of the current is affected, but there is no impact on the shape. The change in current is relatively small. For a change between four

bands and six bands, the maximum divergence is $\approx 5\%$. The change in current with increasing considered bands decreases as we consider additional bands. For example, the difference in current for a calculation accounting for

six versus eight bands is only $\approx 0.3\%$.

VII. REFERENCES

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