Carrier Transport in Bi₂Se₃ Topological Insulator Slab

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Abstract

Electron transport in Bi₂Se₃ topological insulator slabs is investigated in the thermal activation regime (> 50 K) both in the absence (ballistic) and presence of weak and strong acoustic phonon scattering using the non-equilibrium Green function approach. Resistance of the slab is simulated as a function of temperature for a range of slab thicknesses and effective doping in order to gain a handle on how various factors interact and compete to determine the overall resistance of the slab. If the Bi₂Se₃ slab is biased at the Dirac point, resistance is found to display an insulating trend even for strong electron-phonon coupling strength. However, when the Fermi-level lies close to the bulk conduction band (heavy electron doping), phonon scattering can dominate and result in a metallic behavior, although the insulating trend is retained in the limit of ballistic transport. Depending on values of the operating parameters, the temperature dependence of the slab is found to exhibit a remarkably complex behavior, which ranges from insulating to metallic, and includes cases where the resistance exhibits a local maximum, much like the contradictory behaviors seen experimentally in various experiments.

Keywords: Topological Insulator; NEGF; Acoustic Phonons; Quantum Transport; Resistance

1. Introduction

Strong spin-orbit coupling underlies the unique properties of the recently discovered class of novel materials, the three-dimensional (3D) topological insulators (TIs) [1-5], which support the existence of gapless surface states protected by time-reversal-symmetry lying in the insulating band gap of the bulk material. Surface states of a TI can exhibit a single Dirac band with helical-electronic states, i.e. states in which directions of spin and momentum are locked with respect to each other. Such theoretically predicted spin-momentum locking [6, 7] and the robustness of these surface states to non-magnetic impurities [8, 9] has been verified by various experiments, and provides a new basis for potential applications in spin based electronics and optics [10].

Practical device applications of the TIs require that transport be dominated by the topological surface states at room temperature. Here, Bi_2Se_3 with a bulk band gap of ~ 0.3 eV [11, 12] is an attractive candidate, although the pristine Bi_2Se_3 is electron-doped due to the presence of Se vacancies [13], which push the Fermi level into the bulk conduction bands. A variety of methods such as p-type doping [14, 15] and electrical gating [16] have been attempted for the purpose of lowering the Fermi-level so that it lies closer to the Dirac-point. Theoretical analysis suggests that the temperature dependence of resistance in a TI, if transport is dominated by the surface states, would display an insulating trend (resistance decreasing with increasing temperature) [17]. Experimental results on Bi_2Se_3 , on the other hand, show contradictory results in that some experiments observe metallic behavior [16, 18-21], while others find insulating trends [14, 22]. A local maximum in resistance between 100 K and 250 K has also been reported [14-16, 22, 23].

It is clear thus that there is great need to understand the mechanisms underlying transport in TIs in the thermal activation regime, this understanding is also a key for developing applications of TIs. Accordingly, in this study, we attempt a systematic

investigation of how the factors of slab thickness, channel length, Fermi-level (carrier doping), voltage bias, temperature and the strength of electron-phonon coupling [24] compete in a TI in the presence of surface and bulk carriers. This investigation helps in proper understanding of experimental results and a possibility of a new method of detecting surface states via purely electrical transport experiments. Non-equilibrium Green Function (NEGF) approach is used for investigating transport through a slab of Bi_2Se_3 using a realistic model of surface and bulk states. Ballistic transport is considered first, followed by the inclusion of effects of acoustic phonons in the modeling. Our analysis shows that the interplay between various aforementioned factors leads to considerable complexity in the nature of transport in TIs; for example, experimental observation of an insulating trend in a TI need not simply imply operation in surface bands.

This paper is organized as follows. In Section 2, the model used for simulating ballistic and acoustic carrier transport through a Bi_2Se_3 slab within the NEGF framework is presented. Section 3 discusses results for ballistic transport, and it is broken up into several subsections. Subsection 3.1 establishes an operating bias for low field-transport, followed by an evaluation of the temperature dependence of resistance in the thermal activation regime in Subsection 3.2, and a discussion of effects of slab thickness and Fermi-level (E_f) in Subsection 3.3. In Section 4, we bring together various results to provide a more comprehensive understanding of transport in TIs in different regimes of carrier concentration, and discuss how our modeling gives insight into the contradictory experimental observations noted above, by focusing on the effect of channel length and temperature in subsection 4.1 and 4.2 respectively. Section 5 provides a summary of our results and makes a few concluding remarks.

Figure 1. (a) Atomic structure of Bi_2Se_3 . (b) Semi-infinite slab of Bi_2Se_3 with finite thickness along the z-axis and an infinite width along the y-axis. Electron transport is along the x-axis. Gate voltage shifts the Fermi-level (E_f) uniformly in the entire slab. E_f is defined to be zero at the Dirac point. (c) Illustration of potential distribution through the energy bands along the transport direction.

2. Description of Model

Quantum transport through a Bi_2Se_3 slab (see Fig. 1) was modeled for acoustic phonons within the framework of the Keldysh NEGF formalism [25]. Bulk and surface electronic energy bands were described via a $\mathbf{k}\cdot\mathbf{p}$ model and discretized using a finite difference method along the transport direction (x-axis), while the infinitely wide (periodic) transverse direction (y-axis) was modeled using the k-space eigenmodes. This approach has been widely used to simulate an infinitely wide channel with no potential variation along the transverse direction [26, 27] in order to reduce the demand on computational resources [28]. The interlayer coupling was modeled via appropriate real space tight binding parameters. Details of the Hamiltonian are summarized in the Appendix. The key Dirac-cone like surface states is shown as red lines in Fig. 2(a). The local charge distribution, see Fig. 2(b), was

plotted for Dirac bands to quantitatively verify their localization in surface layers. As a further validation of our parameters, the spin textures (see Figs. 2(c) and (d)) of both the top and bottom surfaces were found to display correct chirality. Our parameter set in this way enabled us to simulate transport characteristics manifesting surface as well as bulk behavior.

Figure 2. (a) Energy band structure at $k_y = 0$ for the 13 QL thick Bi_2Se_3 slab. The conduction and valence band edge are at 0.15 eV and -0.15 eV respectively. Red lines give the topological surface bands. (b) Local charge distribution for the surface conduction bands (top surface: blue line; bottom surface: red dashed line) near $k=0$ in different layers of the slab [29]. Note the significant penetration of the surface states into the bulk [30]. (c), (d): In-plane spin-texture of topological surface states around $k=0$ for the top (c) and bottom (d) surface showing their chirality.

The surface Green function was converged iteratively [31] to obtain the self-energy for the source and drain contacts. This emulates perfect contacts with open-boundary

condition. Modeling metallic contacts with hard wall boundary condition [32] for side contacts or even top contacts just modifies the results quantitatively because the current redistributes across the quintuple layers (QL; 1QL ~ 0.943 nm [12]) to flow on both the top and bottom surface layers. Comprehensive analyses of the contact effects for 3D-TI in this work however would be a digression from the fundamental concepts presented in this work and undermine its key points and therefore has been treated elsewhere [33]. Next, the recursive-Green function (RGF) algorithm [34] was applied for calculating the device Green function. Acoustic phonon scattering was modeled as a self-energy [35] to account for momentum relaxation [36]. For the phonon scattering mechanism, deformation potential in the formalism ($\Sigma^{ph} = D_{ac} \cdot \text{diag}(G)$ [36]) was computed from the electron-phonon coupling strength (λ) based on Eq. 27 of Ref. [37], see Appendix A of Ref. [38] for a detailed derivation. However, due to the low-field condition [36], the charge correction arising from Poisson equation was neglected. The experimental values of the Fermi-velocity (v_F) lie over the range of $2.77\text{-}5 \times 10^7$ cm/s [21, 22, 37]. We have used a value of 4.1×10^7 cm/s obtained from slope of surface bands in Fig. 2(a). Temperatures at and above 50 K only were considered in order to capture quantum transport characteristics within the thermal activation regime because the crossover to variable range hopping regime is estimated around 40 K [17]. The current flowing through each layer of the Bi_2Se_3 slab for several values of the Fermi energy around the contact electrochemical potentials in the absence/presence of acoustic scattering of varying strength and other external control parameters was investigated to develop a comprehensive understanding of the transport mechanisms in TIs [39].

3. Ballistic Transport

This section examines ballistic transport through a Bi_2Se_3 slab. The purpose is to delineate appropriate physical conditions for the study of quantum transport, and to also build

a systematic basis for an intuitive understanding of transport as we go from the simpler case of ballistic transport to the more complex behavior when acoustic phonons are included in Section 4 below.

3.1. Source to Drain Bias (V_{DS})

Figure 3. (a) Ballistic I-V characteristics of 13 QL thick Bi_2Se_3 slab at 100 K for Fermi-level (E_f) at Dirac point. Red square is at $V_{DS} = 40$ meV, where the simulations in panels (b)-(f) in this figure have been carried out. (b) Drain current through various layers for four different values (see legend) of V_{DS} . (c) Percentage contribution of various layers to the total drain current for four different values of V_{DS} . Small differences as a function of V_{DS} are not visible in the main plot, and are blown up for layers 1 and 7 in the insets. (d) Surface (bottom layer) and middle (7th layer) layer contribution to the total drain current as a function of for V_{DS} . (e, f) Contribution to the total current from electrons of various energies in different layers (in $\mu\text{A}/\mu\text{m}$) for $V_{DS} = 0.04$ V (e) and 0.16 V (f).

A large voltage might allow electrons to traverse through the bulk bands even if the Fermi-level is tuned to the Dirac point because the current is primarily carried by electrons

with energies lying between the source and drain electrochemical potentials, i.e. between μ_S and μ_D (see Fig. 1). In contrast, at very low voltages, the magnitude of current will be very small and the signal may be masked by the noise floor in a real setup. With this in mind, we simulated low-field transport with bias voltage (V_{DS}) varying from -0.16 V to 0.16 V in a 13 QL thick Bi_2Se_3 slab at 100 K for Fermi-level at the Dirac-point ($E_f = 0$ eV) as a representative case. The results for the total current through the slab are shown in Fig. 3(a), while Figs. 3(b) and (c) show how this total current is distributed among the various layers. In general, the absolute current through each layer in Fig. 3(b) is seen to increase with increasing bias voltage, reflecting an increasing number of electrons contributing to transport. Figure 3(d) shows that the role of bulk bands now starts to increase, which indicates that for high bias, subsurface transport will begin to dominate over surface contribution even when we operate at the Dirac point. This effect will be stronger for thicker slabs as we will see in Section 3.3 below. Figure 3(d) also illustrates that for the positive bias, the bulk contribution scales faster with the increase in the magnitude of V_{DS} compared to a negative bias. This is because most of the electron energies lie in the valence band, where mode density is higher around the Dirac point (see band structure in Fig. 2(a)), compared to the mode density in the conduction band, where most of the Fermi-distribution lie for a negative bias. Furthermore, to justify the choice of 40 mV as an appropriate bias for this study, the energy-resolved current from different layers is presented in Fig. 3(e) and contrasted with the corresponding results at a higher bias of 160 mV in Fig. 3(f). The two color bars are on different scales for better readability. The white (black) regions correspond to the maximum (minimum) current density. The current distribution in Fig. 3(e) illustrates that most electrons flow through the surface layers (1st layer is the bottom surface, 13th layer is the top surface) for energies approaching the average of the contact electro-chemical potentials, corresponding to the maximum in the difference of Fermi-distributions between the source and the drain ($f_{Source} -$

$f_{\text{Drain}} = \Delta f_{SD}$). In Fig. 3(e), the black streaks at 0 and -0.04 eV (-0.16 eV in Fig. 3(f)) reflect the zero density of states (DOS) due to Dirac point at the source and drain ends, respectively. Similarly, dark-red region in the center of the yellowish-white region for surface layers in Fig. 3(f) corresponds to low DOS in the channel (see the potential profile in Fig. 1(c)), resulting in two peaks in energy between μ_S and μ_D . This slight drop in transmission at energy exactly between μ_S and μ_D corresponds to the Dirac-point in the channel and is evident only at high bias or for a long channel device, because the smeared energies in the channel, due to energy level broadening, complemented by non-zero DOS for the contacts at the stated energy level together mask the effect. This point is discussed further in Section 4 below. Note that spread of the dark-red region (also compare the two color scales) on increasing bias in going from Fig. 3(e) to 3(f) shows that the drain current is infiltrated by electrons flowing through bulk states. These considerations justify our choice of 0.04 V as a reasonable bias voltage, which generally limits quantum transport to the surface layers with only minor contribution through the bulk material.

3.2. Temperature

For understanding transport in the thermal activation regime [17], it is important to delineate variations in resistance with temperature, E_f and slab thickness under ballistic conditions. Accordingly, we consider a 13 QL thick Bi_2Se_3 slab over the temperature range of 50 K to 300 K at a bias of 40 mV with $E_f = 0$ (Dirac-point). Figure 4(a) shows that the enhanced thermal activation of the carriers at higher temperatures results in a higher current through the slab. This trend is further seen in the Arrhenius plot in the inset to Fig. 4(a). Even though thermal activation increases the current through each layer in Fig. 4(b), the percentage contribution to the net current in Fig. 4(c) reveals a gradually increasing dominance of

subsurface transport (see Fig. 4(d)), which is not obvious from the absolute current calculations of Fig. 4(b).

Figure 4. (a) Ballistic current as a function of temperature for the 13 QL thick Bi_2Se_3 slab for Fermi-level (E_f) at the Dirac point ($V_{DS} = 0.04$ V). The inset gives an Arrhenius plot of resistance. (b) Drain current through various layers at four different temperatures. (c) Percentage contribution to the total current from various layers at four different temperatures. Differences as a function of temperature are fairly small in the main plot, and are blown up for layers 1 and 7 in the insets. (d) Surface (Bottom layer) and middle (7th layer) layer contribution to the total drain current. (e, f) Contribution to the total current from electrons of various energies in different layers (in $\mu\text{A}/\mu\text{m}$) at $T = 50\text{ K}$ (e) and 300 K (f).

The current distributions in Figs. 4(e) and 4(f) at 50 K and 300 K give insight into the mechanism of increase in subsurface transport at higher temperatures. The yellowish-green region, corresponding to the average of contact electro-chemical potentials, shows that most electrons flow through the surface layers. The red-region in Fig. 4(f) corresponds to the higher energy states, with larger DOS, where the Fermi-distribution is still substantial,

yielding a larger effective current density. Spread of the light blue region along the energy axis for the top and bottom surface layers further exhibits the effect of thermal activation, which corresponds to a spread in the Fermi-distribution for the source and drain contacts. This spread, however, also allows electrons to flow through the bulk bands contributed by the subsurface layers. At 300 K (see Fig. 4(f)), even the bulk valence band of the middle layer contributes to conduction (light blue region in middle-bottom) due to increased hole carrier concentration. By contrast, at the lower temperature of 50 K, much of the conduction remains confined close to the surface.

3.3. Effects of Slab Thickness and Fermi-Level

Figure 5. Variation in ballistic resistance as a function of slab thickness at 100K ($V_{DS} = 0.04$ V) for four different values of the Fermi-level (E_f), see legend.

Bi_2Se_3 slabs, 13 QL to 43 QL thick, were studied at 100 K at a 40 meV voltage bias (V_{DS}) with E_f varying from 0 eV to 0.2 eV, corresponding to the bottom surface carrier density of $\sim 5.62 \times 10^9 / \text{cm}^2$ to $7.21 \times 10^{10} / \text{cm}^2$. This density lies within the experimental range for low carrier doping measurements [14, 18, 21]. In Fig. 5, the experimentally observed

thickness-dependent [19] as well as thickness-independent [20] behavior is reproduced by using different values of the Fermi-level. When the Fermi-level lies in the conduction band (black stars and magenta triangles in Fig. 5), i.e. at high carrier doping, spread of the Fermi-distribution, Δf_{SD} , occurs mainly through the bulk bands, and therefore, conduction increases with increasing thickness of the slab. This is reflected in the steeper slopes in Fig. 5 for higher E_f values, which correspond to higher mode density. However, for the red-squares in Fig. 5, E_f is at the Dirac point, and therefore, for low bias (40 mV) and low temperature (100 K), the spread of Fermi-distribution is mainly concentrated in the surface bands. As a result, despite the increase in the thickness of the slab, conduction remains nearly constant.

Figure 6. (a-d) Ballistic current through various layers for slabs of four different thicknesses, see legend on right hand side of the figure, at 100K ($V_{DS} = 0.04$ V) for different values of the Fermi-levels (E_f) shown on the top of the figure. (e-h) Corresponding percentage contribution to the total drain current.

Further insight is provided by Fig. 6, which shows how the total current is distributed among the various layers as a function of slab thickness for different values of the Fermi

level. When the Fermi-level is set at the Dirac-point in Fig. 6(a), transport is suppressed to virtually zero after a few layers, being confined mainly to the four subsurface layers adjacent to the top and bottom surfaces. This shows that, for $E_f \sim 0$ eV, the surface states dominate transport, and that increasing the thickness of the slab now has little effect on the contribution of the surface layers (see Fig. 6(e)). Comparing the magnitude of current in going from Fig. 6(a) to 6(d), however, we see that the current through various layer approximately scales with E_f or the carrier density (note changes in vertical scale in Fig. 6). When the bulk current is sizeable, increasing the slab thickness reduces the effective contribution of the surface (compare Figs. 6(f)-(h)). Moreover, for higher values of the E_f , even though surface layers have a large contribution, they do not dominate the total current. These results indicate that dominance of the surface layers in conduction can be achieved by fine-tuning the Fermi level to lie close to the Dirac point, or by taking a sample, which is thin enough to reduce the bulk contribution. Fig. 6 should serve as a rough guide for estimating the relative contribution of the surface layer in transport measurements for various carrier densities at the Fermi-level.

4. Acoustic Phonon Scattering

A few experiments have observed an insulating trend in temperature dependent resistance measurements from Bi_2Se_3 samples, similar to the ballistic behavior discussed in the preceding section. However, since the sample length is usually longer than the electronic mean free path (~ 20 nm [40, 41]), the aforementioned trend cannot be associated with ballistic transport. The metallic trend and crossover [14-16, 22] from metallic to insulating behavior has also been observed in the thermal activation regime, which we now turn to discuss.

Acoustic phonons interact with electrons to exchange momentum resulting in the relaxation of electrons, with the resulting scattering strength scaling directly with

temperature. However, at higher temperatures more carriers are excited into the conduction bands leading to an increase in current. Effects of thermal activation and scattering thus compete to determine the overall temperature dependence of resistance. Scattering of electrons, in effect, broadens the density of states, and may equivalently be viewed as a smearing of the energy levels [42, 43]. If the Fermi-level is at the band-edge, an increase in temperature spreads out the Fermi-distribution, leading to a decrease in the carrier density and the magnitude of maxima in Δf_{SD} . However, if the Fermi-level is offset from the band-edge, the spread in Δf_{SD} increases the carrier density (thermal-activation), and the effect of thermal activation gets enhanced. Note that the strength of this effect depends on the relative energy values of the band edge and the Fermi-level, the temperature-dependent spread in the Fermi-distribution, and the strength of acoustic scattering, effects which we now turn to discuss.

4.1. Effect of Channel Length

Figure 7. (a-d) Resistance vs. Channel Length (L_x) for ballistic (red squares) and acoustic transport for weak ($\lambda=0.08$; green triangles) and strong ($\lambda=0.25$; blue star) electron-phonon coupling, for different Fermi-levels at 100 K for 13 QL thick Bi_2Se_3 slab biased at 40mV.

Figures 7(a)-(d) illustrate the effect of channel length on resistance under low-field conditions for different Fermi-levels at a constant temperature. When the Fermi-level ($E_f = 0.2$ eV; Fig. 7(a)) lies in the conduction band, the dominance of in-plane acoustic phonon scattering is demonstrated via constant resistance for ballistic transport and the increase in resistance with channel length seen in the presence of phonons. Impact of the strength of electron-phonon coupling can be seen from the larger slope for $\lambda = 0.25$ (strong coupling) compared to the weak coupling case of $\lambda = 0.08$. However, when the Fermi-level lies in the surface bands close to the bulk band edge ($E_f = 0.1$ eV; Fig. 7(b)), the phonon assisted spread of bulk states enhances the effect of thermal activation, which counters the effect of in-plane phonon scattering. This is evident from the relatively smaller variation in the slopes of resistance versus channel length plots for $\lambda=0.08$ and 0.25 . Next, we consider the case when the Fermi-level lies even closer to the Dirac point ($E_f = 0.05$ eV; Fig. 7(c)). Here, the in-plane acoustic scattering is further weakened, and therefore, slopes of resistance vs. channel length plots are almost the same for two significantly different strengths of electron-phonon coupling. On further reducing doping, to tune the Fermi-level to the Dirac-point, little difference is seen in resistance for different values of λ , but interestingly, resistance increases with channel length for ballistic transport.

Figure 8. Competition between the effects of phonon induced level broadening, thermal activation and in-plane scattering is shown through plots of energy (y-axis) vs transmission, $T(E)$, through the slab, density of states, $DOS(E)$ of the bottom surface in the middle of the channel, and the difference in Fermi-distribution, $\Delta f_{SD}(E)$, between the source and drain for various values of the parameters. Values of $T(E)$ and $\Delta f_{SD}(E)$ are shown on the top horizontal scale (logarithmic) in magenta, while those of the DOS are given on the bottom horizontal scale (logarithmic). *Top Row:* $E_f = 0$ at 100 K for channel lengths (L_x) of 15 nm (a), and 50 nm (b). *Bottom Row:* $E_f = 0.1$ eV, $L_x = 30$ nm at temperatures of 50 K (c) and 250K (d). For better illustration, the values of $\Delta f_{SD}(E)$ are scaled in different panels by the factors given on

the right hand side of each row. $T(E)$ and $DOS(E)$ are scaled up by 2π in all panels. Note that a finer transverse mode grid in the computations will smooth the high energy serrations seen in some of the curves. Red, green and blue colors represent ballistic, weak-acoustic scattering and strong-acoustic scattering cases respectively.

Figures 8(a) and 8(b) further examine these results by comparing the details of transmission (dashed color lines, top horizontal scale) and bottom-surface DOS (solid color lines, bottom horizontal scale) in the middle of the channel for two different channel lengths (15nm and 50nm) for $E_f = 0$ at 100 K to ensure same Fermi-distribution for both cases. The sharp dips in dashed lines show nearly zero transmission at 0 and -0.04 eV energies, indicating the Dirac-points at the source and drain ends. The DOS at energies further from the Dirac-point (closer to bulk states) is larger for the ballistic case (red solid lines), and decreases with increasing scattering strength. On the other hand, the spread of DOS results in larger values of DOS for stronger scattering (green and blue solid lines) in the energy region where Δf_{SD} maximizes (see DOS in energy range between 0 and -0.04 eV), and hence results in high transmission, while phonons reduce transmission at all energies. Next, for the ballistic transport for the longer channel length in Fig. 8(b), a local minimum at -0.02 eV for the transmission (dashed red line) is observed, while there is no such inflection in Fig. 8(a). The reason can be attributed to the Dirac-bands in the source (drain) terminal that have Dirac point at 0 eV (-0.04 eV), and the half V_{DS} drop is assumed in the channel (see Fig. 1(c)) which results in a Dirac point pinned at -0.02 eV in the channel and contributes to minimum surface DOS. For small channel lengths, the DOS from contacts dominate in the transmission, but the weight age of contribution from the channel increases with its length. Therefore, it can be observed that in addition to two dips at the Dirac points of the contacts, transmission at $E = -0.02$ tends to form a local minimum which gets stronger as the channel

length increases. It explains the increasing trend in ballistic resistance seen in Fig. 7(d)., Nevertheless, the phonon induced level broadening further smears the energy level (compare red, green and blue dashed lines in Fig. 8(b)) and overrides the effect of minimum in the channel.

These results give insight into how the Dirac cone states in a TI could be probed via low temperature transport experiments. For this purpose, one would need to measure the resistance of a high quality sample for a range of channel lengths (say from 10-100 nm), in which the Fermi-level is tuned to shift the (expected) Dirac cone to lie between the electrochemical potentials of the contacts. If one finds an increasing trend with channel length, similar to the case of the red curve in Fig. 7(d), that would then suggest the presence of a Dirac cone.

4.2. Effect of Temperature

Figure 9. Resistance vs. temperature for ballistic (red squares) and acoustic transport for weak ($\lambda=0.08$; green triangles) and strong ($\lambda=0.25$; blue star) electron-phonon coupling for four different values of the Fermi-level at 30nm channel length for 13 QL thick Bi₂Se₃ slab biased at 40 mV.

Figure 9 illustrates that when effects of acoustic phonon scattering are included, the temperature dependence of resistivity exhibits a variety of behaviors depending on the specifics of the parameters used. The resistivity is seen to be insulating in some cases, metallic in others, displays a local maximum around 125 K in Fig. 9(c), and a saturation effect in Fig. 9(b), much like the behaviors reported experimentally in various transport measurements on Bi_2Se_3 slabs [14-16, 22]. In Fig. 9(a), ballistic transport results (red squares) are mainly due to thermal activation of electrons regulated by the spread in the Fermi-Dirac distribution, whereas acoustic transport for weak electron-phonon coupling (green triangles) reflects the dominance of phonon scattering, which becomes stronger for larger values of λ (blue stars). We emphasize that our purpose in this study is not to simulate the conditions of any particular experiment, but to provide a framework for obtaining a handle on how different factors play out in transport properties of TIs.

Figure 10. Same as Fig. 8 but for $L_x = 30 \text{ nm}$, $\lambda = 0.25$ for E_f values of 0.05 eV (a) and 0.1 eV (b). Red, green and blue colors represent temperature of 50 K, 125 K and 200 K respectively.

Figure 8(c, d) and Fig. 10 consider interplay of various factors in the overall resistance of the slab by considering the transmission, DOS and Δf_{SD} for various values of the parameters in the simulations. Figure 8(c, d) show that as phonon scattering scales up with temperature, it results in a larger spread of DOS (solid color lines, bottom horizontal scale), and a stronger reduction of transmission (top horizontal scale, note differences in scale in panels (c) and (d)), which generally increases the resistance in Figs. 9(a-c). Nevertheless, as also shown in Fig. 9, for the strong electron-phonon coupling (blue stars), there is a transition from absolutely metallic trend for $E_f = 0.1$ eV (see Fig. 9(b)) to one with a local maxima for lower E_f at 0.05 eV (see Fig. 9(c)), and merits even closer examination of all three effects. Results in Fig. 10 show that in the presence of strong acoustic phonons ($\lambda = 0.25$), as phonon scattering increases with temperature, it induces a decrease in transmission (dashed lines of various colors), and spreads the DOS (solid lines of various colors) and Fermi-distribution over a wider energy range (dotted lines of various colors). The difference in trends between Fig. 10(a) and 10(b) originates from the competition among the three effects at low energies where difference in Fermi-distribution (Δf_{SD}) is low. In Fig. 8(d), a lower transmission throughout the energy grid for higher temperature results in the metallic trend while the spread of Fermi-distribution with increase in temperature in Fig. 10(a), eventually leads to the inclusion of significantly more states for the carriers to traverse the channel and outweighs the effect of transmission. We would also like to note that even though the same Fermi-distribution spread occurs in Fig. 10(b), the contact electrochemical potentials are not at appropriate values (close enough to Dirac-point) to induce the local maxima in resistance trend line. This evinces the importance of relative positioning of the Fermi-level on the energy grid to observe the effect of phonon induced level broadening.

5. Summary and Discussion

Our analysis indicates that an insulating trend of TI resistance measurement vs. temperature is not a sufficient condition for adducing that the Fermi-level in a TI is at or close to the Dirac-point, or that the surface transport is dominant. Such an insulating trend only indicates that the overall effect of electron-phonon coupling is weaker than that of thermal activation under the operating conditions. A more detailed understanding of the material specific electron-phonon coupling strength and other factors discussed above is needed for a reliable interpretation of the experimentally observed temperature dependence of the resistivity in the TIs.

Finally, since most experiments have seen metallic behaviour, for understanding purpose and gaining top level insight into peculiar resistance behaviour, it may be useful to compare 3D-TI with normal metals which universally show increase in resistance with temperature. In TI literature, ‘insulator-like’ trend is referred to increasing resistance with decreasing temperature, whereas decreasing resistance trendline is termed metallic trend. This is because in metals, due to phonon scattering, the resistance increases with temperature. In normal metals, Fermi-level (E_f) is already well above the conduction band edge and therefore the effect of small increase in carrier density due to thermal activation is easily masked by phonon scattering whose strength scales directly with temperature. However, for insulators, provided E_f , although below conduction band edge, if it is still in purview of thermal activation energy, more electrons can populate conduction band as the temperature is increased which results in decreased resistance. To put it simply, the Dirac-bands and phonon scattering in 3D-TI provide an interesting competition between these effects. For Dirac-bands, Density of states increases linearly with energy (referenced w.r.t Dirac point), and therefore as electrons populate higher energies current should increase, however weighted by the Fermi-Distribution function. Therefore, in absence of phonon scattering (ballistic

transport) resistance always decreases with increasing temperature. In fact when operating close to the Dirac point for 3D-TI, we show that still phonon scattering cannot override the thermal activation into higher energies and hence insulating trend is observed. However, as E_f gets closer to the bulk bands, resulting in electronic condition similar to metals, the phonon scattering transcends the overall characteristics. Moreover, this transition should result in local maxima in resistance vs temperature trendline as observed in some of the experiments.

In summary, we discuss electronic transport in a Bi_2Se_3 slab as an exemplar TI system in the thermal activation regime (> 50 K). Our modeling includes effects of acoustic phonons in the presence of bulk and topological surface states. Resistance is computed within the framework of the NEGF formalism. Simulations are carried out for a range of values of electron-phonon coupling strength, slab thickness, channel length, Fermi-level (carrier doping), voltage bias across the slab and temperature. In this way, we show how the interplay between the competing effects of thermal activation, phonon induced level broadenings and in-plane scatterings can yield quite complex temperature dependencies of the overall resistivity of the slab. When the Bi_2Se_3 slab is biased at the Dirac point, the temperature dependence of the resistance is found to display an insulating behavior even in the case of strong electron-phonon coupling strength. However, when the Fermi-level lies within or close to the bulk conduction band (heavy electron doping), phonon scattering dominates and results in a metallic behavior, although the insulating trend is retained in the limit of ballistic transport. Depending on operating conditions, resistance of the slab can thus exhibit a metallic or an insulating character or a local maximum in resistance as a function of temperature, much like the types of contradictory trends seen in various experimental measurements. Our study provides a systematic basis for understanding aspects of the complex transport properties of TIs and their dependencies on various operating parameters needed for practical exploitation of the topological surface states in potential applications of

the TIs. Further extensions of our modeling to account for effects of surface relaxations, environmental degradation of the sample, and transverse mode couplings and scatterings to treat nanowire systems would be interesting.

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Appendix: Electronic structure model of Bi_2Se_3

Our effective Hamiltonian for each quintuple layer is:

$$H_p = \begin{bmatrix} k^2/m_1 & d+k^2/m_2 & ivk_x - vk_y & 0 \\ d+k^2/m_2 & k^2/m_1 & 0 & -ivk_x + vk_y \\ -ivk_x - vk_y & 0 & k^2/m_1 & d+k^2/m_2 \\ 0 & ivk_x + vk_y & d+k^2/m_2 & k^2/m_1 \end{bmatrix}, \quad (\text{A.1})$$

where v is the velocity parameter, m_1 and m_2 are the orbital masses, and d is the hopping between the two same-spin orbitals within the quintuple layer [44]. The hopping between two adjacent quintuple layers is given by

$$T = \begin{bmatrix} 0 & 0 & 0 & 0 \\ t_z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & t_z & 0 \end{bmatrix}, \quad (\text{A.2})$$

where t_z is the nearest neighbor hopping parameter. The total Hamiltonian for a Bi_2Se_3 (semi-infinite) slab can then be written as

$$\overline{H} = \begin{bmatrix} H_1 & T_1 & & 0 \\ T_1^\dagger & H_2 & T_2 & \\ & T_2^\dagger & H_3 & \\ 0 & & & \ddots \end{bmatrix}, \quad (\text{A.3})$$

where $H_i = H_p$ and $T_i = T$ where i is the index of quintuple layers. We have $m_1 = 0.125 \text{ eV}^{-1}\text{\AA}^{-2}$, $m_2 = -0.04 \text{ eV}^{-1}\text{\AA}^{-2}$, $d = -0.22 \text{ eV}$, $v = 2.5 \text{ eV}\text{\AA}$, and $t_z = 0.35 \text{ eV}$. Values of these parameters are chosen to yield a semiconducting gap $\sim 300 \text{ meV}$ for Bi_2Se_3 to simulate the single-Dirac-cone topological surface states. The model, however, does not describe the hexagonal warping, which manifests itself mainly at energies higher than 0.435 eV above the Dirac point in Bi_2Se_3 . In particular, ARPES results on Bi_2Se_3 show approximately isotropic energy contours up to 250 meV above the Dirac point (see Fig 2(e) of Ref. [45]), while this is not the case in Bi_2Te_3 (see Fig. 1(b) of Ref. [46]), and therefore, this energy regime is very well captured by our model.

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