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Band-Alignment Induced Current Modulation in Bi_2Se_3 Topological Insulator

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Abstract

Band alignment induced current modulation in Bi_2Se_3 three-dimensional (3D) topological insulator (TI) slab has been investigated by quantum transport simulations, implemented through Non-Equilibrium Green Function (NEGF) formalism, to examine the possibility of a 3D-TI based resonant device for future spintronic oscillators and analog multipliers. It is observed that maximum current flows when the Dirac-points (bands) are in resonance. However, On/Off ratio is found to be relatively small and strong temperature dependence is also noticed. The physical insights for these observations have been posited along with the suggestions for attaining close to ideal operation.

1. Introduction

Single gapless linear Dirac bands on the surface of 3D-TI [1], with bulk insulating phase, are protected by time-reversal symmetry against any non-magnetic perturbation [2] to ensure high conductivity because of suppression of backscattering. Furthermore, spin-momentum locking [3] for carrier transport in these helical surface states projects TI as a promising candidate for spintronic applications [4]. Among the extant 3D-TI, Bi_2Se_3 [5] has the largest bulk bandgap of 0.3 eV which provides large energy window for exploiting these exotic surface states, and hence has been chosen as representative material in this work.

Leveraging on the Dirac-bands of graphene, recently there has been a proposal of symmetric Field Effect Transistor (SymFET) [6], a novel device with a resonant current peak for an appropriate balance of channel bias (V_{DS}) with Fermi-level (E_f). This device based on vertical tunneling from n-doped layer to p-doped layer, separated by an insulator, is expected to exhibit a large current switching ratio which is symmetrical about resonant peak, at which the Dirac-points (bands) exactly align between two layers (c.f. Fig. 4(b) of [6]), and independent of temperature variation. Consequently, SymFET has been considered as a candidate for the applications to high-speed analog multipliers and oscillators [6].

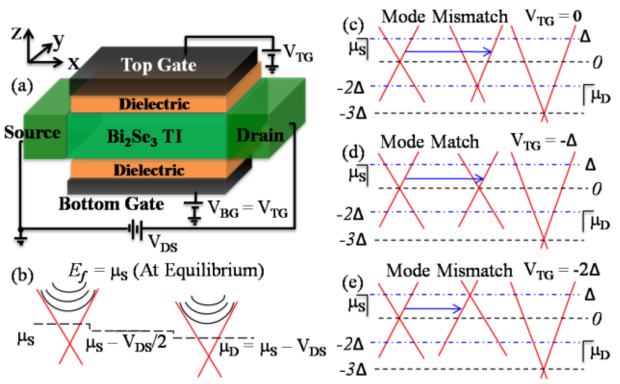

Fig. 1. (a) Device Structure for quantum transport modeling through Bi_2Se_3 slab with shorted top and bottom gates. (b) Potential distribution through the energy bands along the transport direction. μ_S (μ_D) is electrochemical potential at source (drain) end. (c, d, e) Schematic of band profile along the transport direction (source, channel and drain from left to right) for three different gate voltages, illustrating the mechanism of mode matching. For 0K, transport is within the energy window delineated with blues dot-dashed line. Blue arrows depict ballistic transport along the transport direction with conserved transverse momentum.

In this work, therefore, we examine the possibility of a similar band-alignment induced switching operation, but for lateral transport, in 3D-TI device which may serve as an analogue of multipliers and oscillators in spintronic circuits. We observed that although there is a resonant peak due to mode matching, the switching ratio is relatively small and device transfer characteristics depend on temperature. We expound the device mechanism to elucidate the limiting factors and provide suggestions to improve the device performance.

2. Methodology

Fig. 1(a) illustrates the device structure with 13 quintuple layer (QL) (1 QL ~ 0.943 nm) thick (z-axis) TI slab (infinite along y-axis modeled with uncoupled mode space approach) of 20 nm channel length (x-axis) with semi-infinite contact on either side of the channel. The potential profile along the transport direction is shown in Fig. 1(b) for a de-facto fully n-doped device. Ballistic quantum transport through the defect-free device is modeled via NEGF using device Hamiltonian extracted from ab-initio calculations in Ref.[7]. Self-energy for contacts has been computed self-consistently. Dual gates (shorted), with translation factor of unity, on top and bottom ensure uniform effect on all the layers of TI in the channel. A channel bias of $V_{DS} = 2\Delta$ (see Fig. 1) has been applied across the device. Bands are shifted by applying the gate voltage (V_{TG}), which is swept from 0 (n-doped) to -2Δ (p-doped) (see Fig. 1(c-e)). The resonant condition, in this structure is expected at $V_{TG} = -\Delta$ at which the Dirac-point in source and channel align together.

3. Results and Discussion

Fig. 2 illustrates the clear evidence of resonant current peaks, in transfer characteristics of the device for different Fermi-levels, which can indeed be employed for spintronic analog circuits. As expected, current increases with increasing magnitude of E_f because of operation in larger density of states (DOS) region which scales linearly with energy for Dirac bands. The shift in the resonance point which universally occurs at $V_{TG} = -\Delta$ is another evidence of

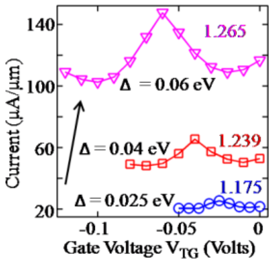

Fig. 2. Device operation for three different Fermi-Levels ($E_f = \Delta$ at equilibrium, FIG. 1) in surface bands (V_{DS} = 2 Δ) at 0K. On/Off ratio is defined between V_{TG} = 0V (Off state) and V_{TG} = - Δ (On State) and stated over each trendline with respective color. Note the resonant peak and its translation along the gate-voltage axis with Δ.

band-alignment effect. However, there are three additional observations from the quantum transport. Firstly, the current at two extremes of V_{TG} (0 and -2Δ) is not equal (higher at V_{TG}=0). Secondly, there is a local minimum on either sides of resonance. Thirdly, the current in off state (V_{TG} = 0) is not negligible. The first happens because of mode-mismatch between bands in channel and drain and therefore is strongest for V_{TG} = -2Δ. The effective DOS in the transport energy window between μ_S and μ_D (see Fig. 1) is responsible for second observation. As the V_{TG} is swept from 0 to -Δ, it starts to move the higher DOS out of energy window and replaces it with lower DOS, which results in continuous decrease in current. DOS again increases from –Δ onwards. However, the effect of DOS competes with the mode matching between source and channel, the fundamental mechanism of band-alignment device. To closely examine the cause for third one, transmission spectrum has been plotted in Fig. 3. It clearly illustrates the physics of band-alignment with symmetric operation about Dirac-point for V_{TG} = -Δ and maximum mismatch when carriers have to traverse from conduction to valence band or vice versa. Note that for non-equilibrium transport, only the transverse momentum (ky wave-vector) must be conserved. Conservation is not required along transport direction (kx wave-vector). In fact this is the reason that vertical tunneling (along z-axis) Graphene symFET is expected to have strong resonant peak because both kx and ky wavevectors must be conserved allowing only for only one energy point for transport and hence better mode selectivity. Non-zero

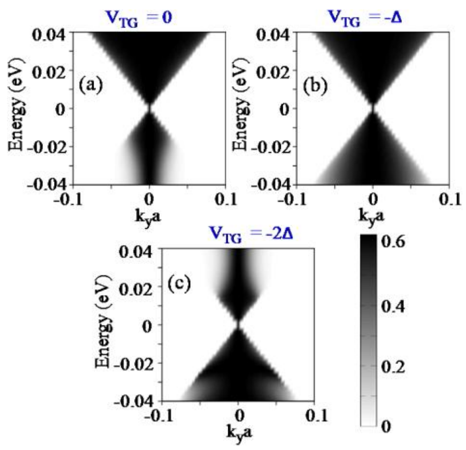

Fig. 3. Transmission spectrum (per μm) at Δ = 0.04 eV for V_{TG} corresponding to schematics in Fig. 1(c, d, e) at 0K.

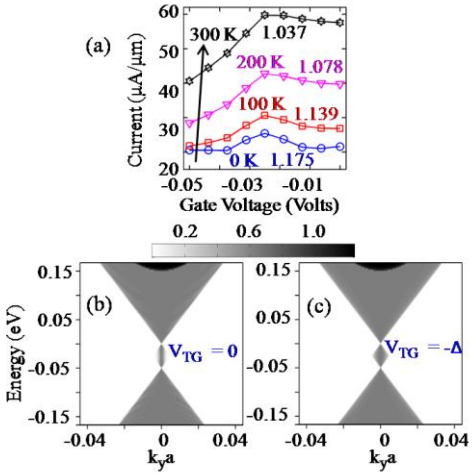

Fig. 4. (a) Current at four temperatures for Δ = 0.025eV. On/Off ratio and temperature are stated with respective colors for each trendline. Observe that signature of mode matching is severely weakened due to spread in Fermi-distribution. (b, c) Transmission spectrum (per μm) for two gate voltages at 300K. Compare it with Fig. 3 to observe the extinction of signature of mode match/mismatch in quantum transport. Dark black region is first bulk conduction band.

transverse multi-modes in our device result in nearly complete loss of resonance at 300K as illustrated in Fig. 4 by plotting both transfer characteristics and transmission spectrum. Therefore, to improve the performance there is a need to implement mode selective switch in the channel to completely filter out the non-normal modes (ky ≠ 0), for instance by putting tilted gates or an insulating physical barrier like a lens in the channel [8]. Heterostructures [9] or exact symFET [6] architecture are other possibilities which can be investigated in future work.

4. Conclusion

We have examined the feasibility and performance of a resonant device for Bi_2Se_3 3D-TI, a spintronic material. It is found that switching ratio is not very exciting atleast for the simple structure considered in this work which is the first to appraise such a possibility. The degradation of the ratio is chiefly because transport in non-resonant condition is not exactly limited to one energy point between contact electro-chemical potentials (μ_S and μ_D) as may be expected for Graphene symFET. Therefore, we have suggested exploring solutions to limit the transverse modes for improving the device performance.

Acknowledgments

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