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Carrier transport in Bi_2Se_3 topological insulator slab

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ABSTRACT

Electron transport in Bi_2Se_3 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 Bi_2Se_3 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.

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 $\sim$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.

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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. Section 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 Section 3.2, and a discussion of effects of slab thickness and Fermi-level (E_f) in Section 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 Sections 4.1 and 4.2 respectively. Section 5 provides a summary of our results and makes a few concluding remarks.

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 k•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 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 Fig. 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.

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 ($\Sigma^{ph} = D_{ac} \bullet diag(G)$ [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 $2.77 - 5 \times 10^7$ 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

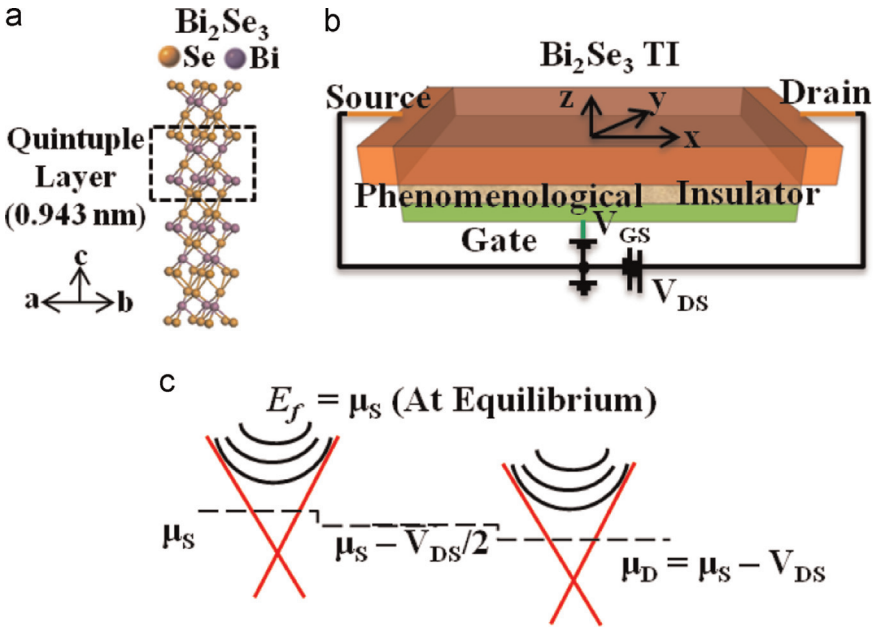

Fig. 1. (a) Atomic structure of Bi_2Se_3. (b) Semi-infinite slab of Bi_2Se_3 with finite thickness along the z-axis and an infinite width along *the* y-axis. Electron transport is along the x-axis. Gate voltage shifts the Fermi-level (E_f) uniformly in the entire slab. E_f is defined to be zero at the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