NEMO5: Why must we treat topological insulator nanowires atomically?

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INTRODUCTION

Surface electrons in topological insulator (TI) based devices such as Bi_2Te_3 nanowires face no backscattering in the absence of magnetic impurities. Their surface conductance is expected to be only limited by the surface Fermi velocity [1]. However, experimental values of the Bi_2Te_3 surface Fermi velocity varies more than 10% [2, 3].

So far, theoretical studies of TI wires assume rotational symmetry along the wire axis. In the case of Bi_2Te_3 this assumption is only true for wires grown along [001] direction [4]. In contrast, fabricated Bi_2Te_3 nanowires are grown in [110] direction and often have rectangular cross sections [5]. The facets of [110] Bi_2Te_3 nanowires show different chemical compositions: Two facets are composed of Te atoms only and the other two contain both Te and Bi atoms. Such details of the surface chemistry require atomistic representations.

In this work, atomistic sp3d5s* (20 band) tight binding bandstructure calculations of Bi_2Te_3 nanowires are presented. In agreement with Ref. [4] the band gap of the Bi_2Te_3 nanowires close in this work when the magnetic flux through the wire cross section agrees with half-integer flux quanta. Deviations from literature are found in the details of the surface state energies and surface Fermi velocities: Fermi velocities of chemically different surfaces differ. This creates an effective potential on the wire surface which can confine TI surface states on specific surface facets. Guided by the atomistic results, the analytical Fermi velocity model of Ref. [4] is augmented to cover the impact of the detailed wire surface chemistry.

MODEL

In this work, atomistic sp3d5s* (20 band) tight binding bandstructure calculations of Bi_2Te_3 nanowires are calculated by the multipurpose NanoElectronics Modelling Tool (NEMO5) [6]. Magnetic fields are included in terms of the Peierl's phase factor in symmetric gauge [8]. All presented atomistic calculations are numerically very intense and required typically about one million CPUs on the Blue Waters supercomputer. The surface bandstructures of these sophisticated results are very well fit with a new analytical model. This model is an extension of the one in Ref. [4] to include different Fermi velocities on different wire facets.

RESULTS

The atomistic tight binding model with the Peierl's phase factor of NEMO5 reproduces the band gap dependence on magnetic fields as discussed in Refs. [4] The calculated oscillations of the magnetoconductance in these nanowires for different gate voltages agree qualitatively with experimental data of Ref. [5] (see Fig.1). One dimensional helical states are observed in the wires agreeing with Ref. [7] (see Fig.2). Figure 3 illustrates differences in the bandstructures of rectangular Bi_2Te_3 nanowires with different ratios of pure Te and mixed atom type surfaces. The surface states of these atomistic calculations are subject to confinement depending on the facet's dimension and chemistry.

The surface bandstructures of the atomistic calculations serve as fitting targets for the surface Fermi velocities of the new analytical model. The analytical model can efficiently predict effective surface potentials which confine surface states on specific facets.

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CONCLUSION

In summary, the atomistic representation of Bi_2Te_3 wires unveils chemically different wire surfaces and surface state dispersion relations. The presented analytical model is able to predict the atomistic results for the surface state dispersion and confinement.

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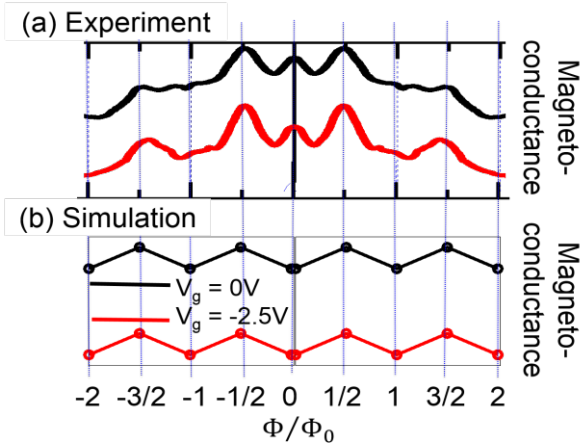

Fig. 1. (a) Experimental Magnetoconductance as function of magnetic flux Φ in units of magnetic flux quanta $\Phi_0 = h/e$ for magnetic fields applied parallel to the axis of the nanowire in Ref.[5] at two different gate voltages. NEMO5 simulation results (b) agree qualitatively with (a).

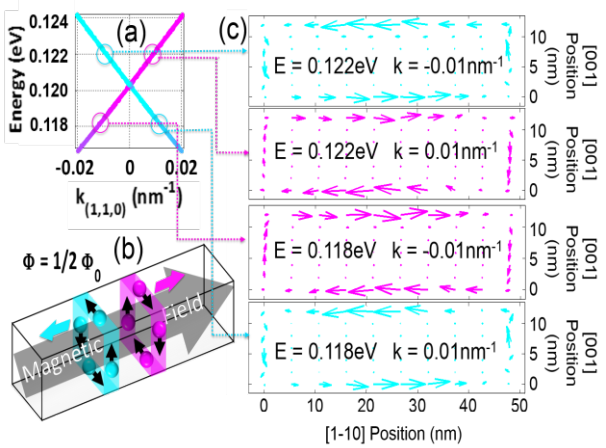

Fig. 2. 1D helical surface states of a 48x12nm^2 Bi_2Te_3 nanowire with a magnetic field of 3.5949T solved with NEMO5 for the two (E,k) tuple as indicated in the bandstructure in (a). The color represents different spin orientations in (b). Electrons of the same energy and opposite spin orientation propagate into opposite direction as illustrated in (c).

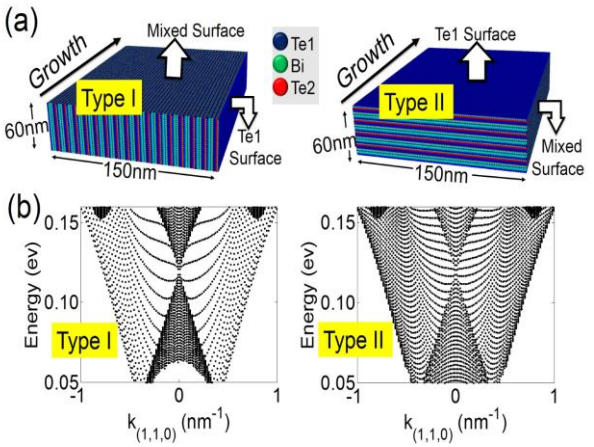

Fig. 3. (a) Atomic structures of 60x150 nm^2 Bi_2Te_3 nanowires grown along the 110 direction. The facets with only Te1 atoms are larger in type I than in typeII wires. (b) Bandstructures of the nanowires of (a).

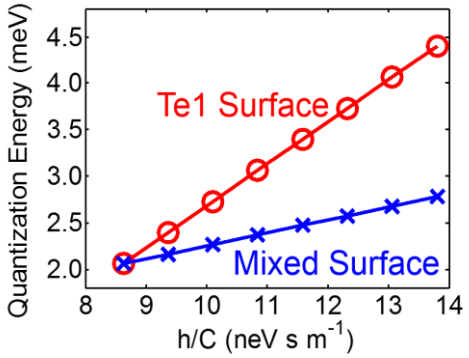

Fig. 4. Surface state quantization energies as a function of the inverse wire circumference C for Bi2Te3 nanowires grown in [110] direction. Different facets of [110] wires differ in their chemistry and give different quantization energies. Surface Fermi velocities can be extracted from linear fits to these data.