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\textsubscript{2}Te\textsubscript{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 \cite{1}. However, experimental values of the Bi\textsubscript{2}Te\textsubscript{3} surface Fermi velocity varies more than 10\% \cite{2, 3}.

So far, theoretical studies of TI wires assume rotational symmetry along the wire axis. In the case of Bi\textsubscript{2}Te\textsubscript{3} this assumption is only true for wires grown along [001] direction \cite{4}. In contrast, fabricated Bi\textsubscript{2}Te\textsubscript{3} nanowires are grown in [110] direction and often have rectangular cross sections \cite{5}. The facets of [110] Bi\textsubscript{2}Te\textsubscript{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 sp\textsuperscript{3}d\textsuperscript{5}s\textsuperscript{*} (20 band) tight binding bandstructure calculations of Bi\textsubscript{2}Te\textsubscript{3} nanowires are presented. In agreement with Ref. \cite{4} the band gap of the Bi\textsubscript{2}Te\textsubscript{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. \cite{4} is augmented to cover the impact of the detailed wire surface chemistry.

MODEL

In this work, atomistic sp\textsuperscript{3}d\textsuperscript{5}s\textsuperscript{*} (20 band) tight binding bandstructure calculations of Bi\textsubscript{2}Te\textsubscript{3} nanowires are calculated by the multipurpose NanoElectronics Modelling Tool (NEMO5) \cite{6}. Magnetic fields are included in terms of the Peierl’s phase factor in symmetric gauge \cite{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. \cite{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. \cite{4} The calculated oscillations of the magnetoconductance in these nanowires for different gate voltages agree qualitatively with experimental data of Ref. \cite{5} (see Fig.1). One dimensional helical states are observed in the wires agreeing with Ref. \cite{7} (see Fig.2). Figure 3 illustrates differences in the bandstructures of rectangular Bi\textsubscript{2}Te\textsubscript{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.
CONCLUSION

In summary, the atomistic representation of Bi$_2$Te$_3$ 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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REFERENCES