

Full band electron band structure calculation with empirical tight binding for topological insulators and broken gap devices

Parijat Sengupta, Tillmann Kubis, Michael Povolotskyi, and Gerhard Klimeck
 Network for Computational Nanotechnology, Purdue University, Indiana 47907, USA
 e-mail: psengupta@purdue.edu

INTRODUCTION

Many modern semiconductor devices and materials yield band structures that do not allow a distinction between electrons and holes. Primary examples of such devices and materials are broken-gap super-lattices, band-to-band tunneling diodes and topological insulators [1,2]. Reliable theoretical predictions of the device performance, when a finite voltage is applied require charge self-consistent band structure calculations. Andlauer and Vogl developed a charge self-consistent k.p envelope-function method that avoids the concept of holes [3]. Modern devices, however, are often too small for envelope-function methods and atomistic descriptions become inevitable. This work continues the concept of Ref. [3] and introduces a novel charge self-consistent full-band atomistic tight binding method that avoids usage of holes. To demonstrate this method, the charge self-consistent band structure of a 6nm thick Bi_2Te_3 layer is calculated. This method is also applicable to transport calculations in band to band tunneling structures and broken gap devices (implemented within NEMO5 [4]).

METHOD

The central concept of this method is to consider every eigen state of the full band tight binding Schrödinger equation as an electronic state. Occupation of these states is given by a Fermi distribution. The electron density on every atom is defined as the product of the squared absolute value of the eigen state amplitude and its occupancy probability, summed over all states. Each material's atom is addressed an ion charge that depends on the specific tight binding model

and the corresponding material parameterization. To define this ion charge, the Schrödinger equation of the bulk material is solved; the resulting atom-resolved electron density is assumed to agree precisely with the ion charge density of opposite polarity. This guarantees that the charge self-consistent bulk band structure is in complete agreement with the empirically determined parameterization. The total space charge on every atom node is a sum of atomically resolved electron densities and the material dependent ion charges. Since all tight binding valence bands contribute explicitly to the density calculation, the dielectric constant of the Poisson equation is set to unity.

RESULTS

All results are produced with NEMO5 [4]. The method is applied to the topological insulator Bismuth Telluride (Bi_2Te_3) in the $\text{sp}^3\text{d}^5\text{s}^*$ basis representation [5]. The bulk band structure of Bi_2Te_3 is given in Fig.1. Positive ion charges of 3.898e for Bi, 6.521e for Te1 and 7.159e for Te2, are determined. These parameters are used to solve the spin resolved band structure of a 6nm thick Bi_2Te_3 layer grown in (100) direction. The two surfaces are terminated with Bi and Te2, respectively. The charge self-consistently calculated electrostatic potential and the space charge density are shown in Figs.2 and 3 respectively. The electrostatic potential in Fig.2 is a correction to the electron-electron interaction already covered by the empirical tight binding parameters and therefore maintains a smooth shape. Figure 4 illustrates the self-consistent spin resolved band structure. It shows two Dirac cones and spin polarizations along the growth axis that are typical of topological insulators [1].

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REFERENCES

- [1] A. Bernevig, T. Hughes, and S. Zhang, *Science*, 314, 1757-61 (2006).
- [2] W. Shan, H. Lu, and S. Shen, *New Journal of Phys* 12 (2010) 043048
- [3] T. Andlauer, and P. Vogl, *Phys. Rev. B* 80, 035304 (2009)
- [4] S. Steiger *et al.* *IEEE Trans. on Nanotech*, Vol10, pg.1464 (2011)
- [5] S. Lee, and P. Allmen, *Appl. Phys. Lett.* **88**, 022107 (2006)

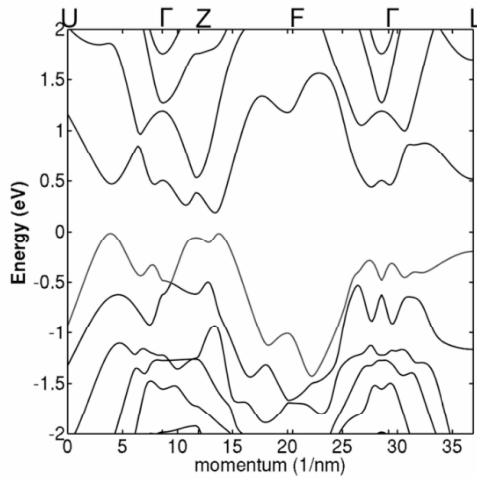


Fig. 1. Bulk band structure of bismuth telluride according to the parameterization of Ref. [5].

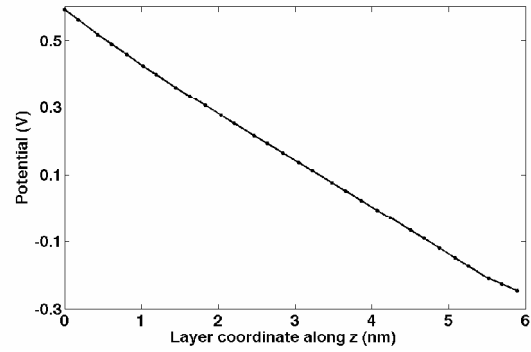


Fig. 2. Charge self-consistent electrostatic potential profile across a 6nm thick Bi_2Te_3 layer. The Bi terminated surface is at $z=0$, the surface at $z=6\text{nm}$ is terminated with Te_2 .

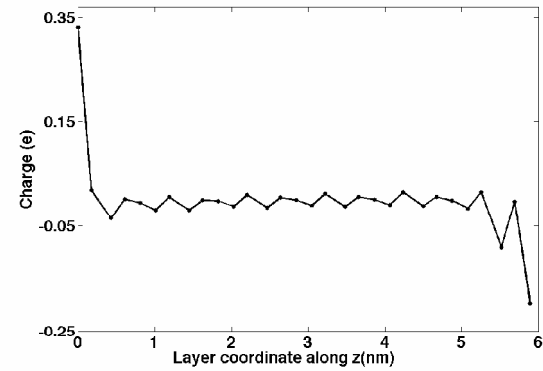


Fig. 3. Space charge distribution self-consistent with the potential profile shown in Fig. 2. The two interfaces at $z=0$ and $z=6\text{nm}$ show charge buildup of opposite polarity.

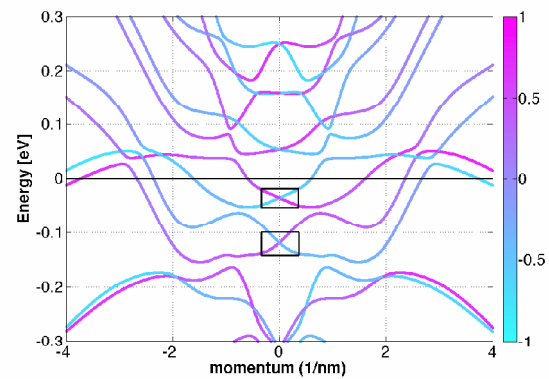


Fig. 4. Dispersion of the bismuth telluride layer of Fig. 2 in (010) direction. Colors indicate the spin polarization in the growth direction. The black boxes mark the Dirac points of the TI surface states.