Symmetry-Based Modeling of Topological Crystalline Devices

B. Dellabetta*, C. Fang*, A. Pecchia†, A. Di Carlo†, B.A. Bernevig‡, and M.J. Gilbert*
*Micro and Nano Technology Laboratory, University of Illinois at Urbana-Champaign, USA
†Department of Electronic Engineering, University of Rome, Tor Vergata, Rome, Italy
‡Department of Physics, Princeton University, New Jersey, USA
e-mail: matthewg@illinois.edu

INTRODUCTION

Topological insulators (TIs) have emerged as an interesting new class of 3D materials that possess spin-momentum locked surface states protected from backscattering by time-reversal symmetry (TRS) [1]. However, to date few applications have been proffered that take advantage of these unique properties beyond attempts at field-effect transistors [2].

Recent theoretical work, however, has shown that TRS-protected TIs are just one type in a wide field of topological materials. One such class, topological crystalline insulators (TCIs), are protected by point-group symmetry (PGS) and are much more conducive to possible semiconductor device and quantum computing applications.

In this work, we focus on the rock-salt $Pb_{1-x}Sn_xTe$ that has been theoretically [3] and experimentally [4] shown to possess topologically nontrivial low-energy surface states occurring near the $\bar{X}$ and $\bar{Y}$ high-symmetry points of the Brillouin zone, as shown in Fig. 1. The topological band crossings in this material are protected by mirror symmetry.

MODEL

We use the inherent symmetry of SnTe to derive a simple 2D $k \cdot p$ model that captures the correct spin-texture for the TCI near the Dirac cones,

$$H(\vec{k}) = v_0 k_x \sigma_0 + v_1 k_x \sigma_2 + v_2 k_y \sigma_1, \qquad (1)$$

with material parameters $\{v_0, v_1, v_2\} = \{0, 1.1, 2.8\}$ eV$\cdot\mathring{A}$. σ denote Pauli matrices, with σ_0 the identity matrix. We also extend the symmetry argument to derive a simple 3D tight-binding model that accurately reproduces the band structure. While simple in its derivation, we find that the 3D symmetry-based model is insufficient to reproduce the known spin-texture of the TCI. We will discuss a more complete tight-binding model which accurately captures both the spin and charge dynamics.

DISCUSSION

We utilize the 2D model in Eq. 1 to study a TCI transistor whose state is switched from "on" to "off" via strain induced by a field deformed piezoelectric. The band structure is shown in Fig. 2. Strain can be applied to the model to break PGS and open a gap, such that the TCI can be used as a topological switch, with quantized conductance shown as a function of strain in Fig. 4.

We plot the DOS of the 3D model along the top surface near $\bar{X}$ in Fig. 3. As chemical potential increases, Dirac cones on either side of $\bar{X}$ manifest a Lifshitz transition, in which the topology of the Fermi surface changes. The 3D model captures the correct TCI band structure, but further additions to the 3D model are necessary to properly mimic spin-texture and determine viable transport phenomena for spintronic applications.

REFERENCES

[1] M.Z. Hasan and C.L. Kane *Colloquium: Topological Insulators*, Review of Modern Physics **82**, 3045 (2010).
[2] H. Zhu et al. *Topological Insulator Bi_2Se_3 Nanowire High Performance Field-Effect Transistors*, Scientific Reports **3**, 1757 (2013).
[3] T.H. Hsieh et al. *Topological crystalline insulators in the SnTe material class*, Nature Communications **3**, 982 (2012).
[4] S.-Y. Xu et al. *Observation of a topological crystalline insulator phase and topological phase transition in $Pb_{1x}Sn_xTe$*, Nature Communications **3**, 1192 (2012).

ISBN 978-2-9547858-0-6

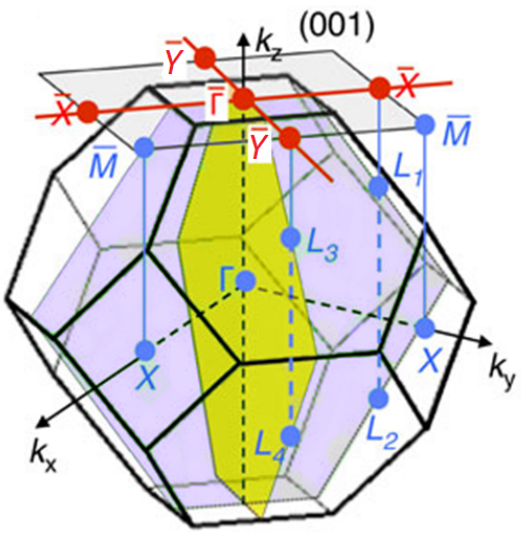

Fig. 1. Rocksalt lattice structure and 3D Brillouin zone of $Pb_{1x}Sn_xTe$. Adapted from [4].

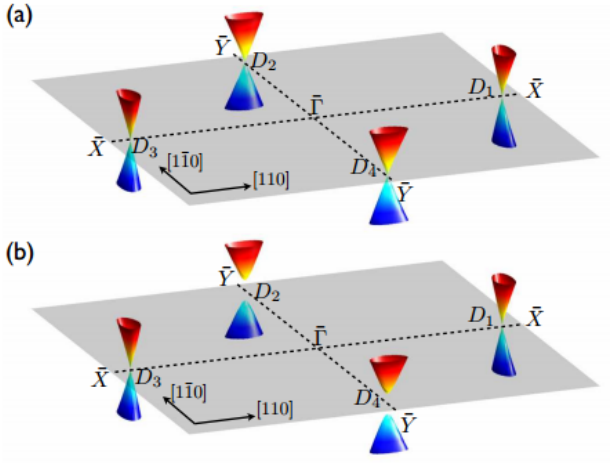

Fig. 2. (a) 2D Brillouin zone along the (001) surface. Gapless surface states emerge on either side of $\bar{X}$ and $\bar{Y}$. (b) Strain in the (111)-direction opens a gap in Dirac cones D_2 and D_4, about $\bar{Y}$.

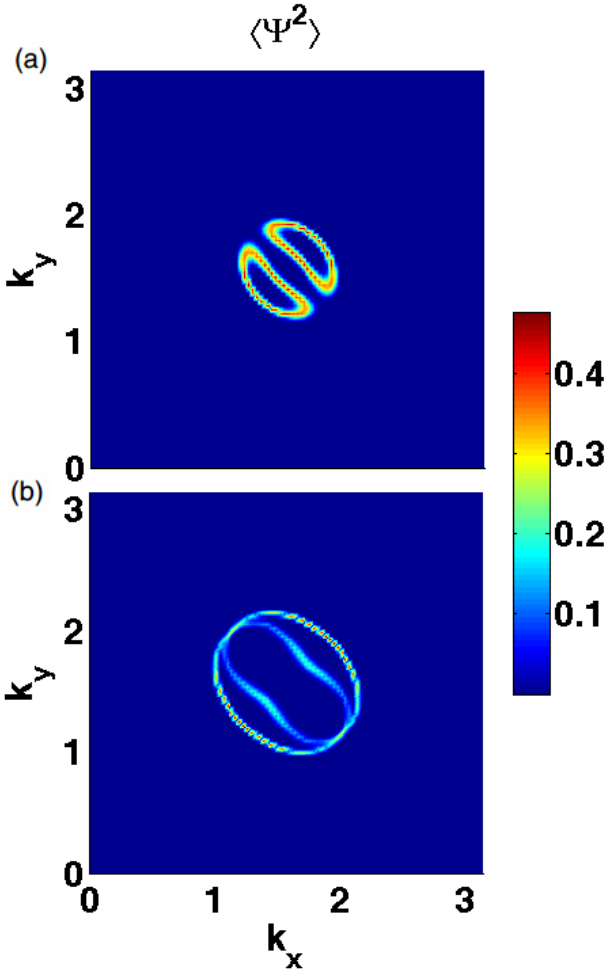

Fig. 3. Local DOS on the surface of SnTe for (a) $\mu = 0.16$ eV and (b) $\mu = 0.48$ eV. $\bar{\Gamma}$ and $\bar{X}$ are located at (0,0) and $(\frac{\pi}{2}, \frac{\pi}{2})$, respectively.

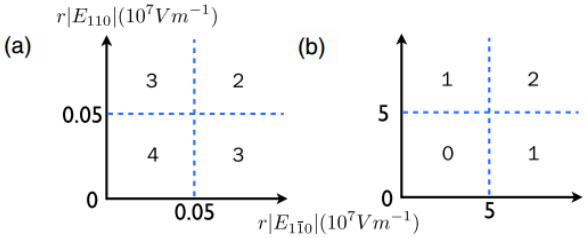

Fig. 4. Quantized conductance (units of e^2/h) in TCIs in the (a) thick (>20 nm) and (b) thin film (5-10 nm) limit.