DOE Final report-2012-2016

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Project Title: STM Studies of Spin-Orbit Coupled Phases in Real- and Momentum-Space
Name of the PI: Vidya Madhavan
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Period covered by the report: 4 years, from 07/14/2012 to 07/31/2016

Description of accomplishments

1. **Coexistence of massless and massive Dirac fermions in topological crystalline insulators (TCIs).** Published in ***Science*** 341, *1496-1499* (2013)

In the recently discovered topological crystalline insulators, topology and crystal symmetry intertwine to create surface states with a unique set of characteristics. Among the theoretical predictions for TCIs is the possibility of imparting mass to the massless Dirac fermions by breaking crystal symmetry. In this work we carried out high resolution scanning tunneling microscopy studies of a TCI, $Pb_{1-x}Sn_xSe$. Using Landau level spectroscopy, we discover the existence of zero mass Dirac fermions coexisting with massive Dirac fermions in TCIs (Fig.1). Our theoretical model shows that this is consistent with broken mirror symmetry in one direction leading to the first experimental proof that the Dirac node in TCIs is protected by mirror symmetry. Our work paves the way for engineering the Dirac band gap and realizing interaction-driven topological quantum phenomena in TCIs.

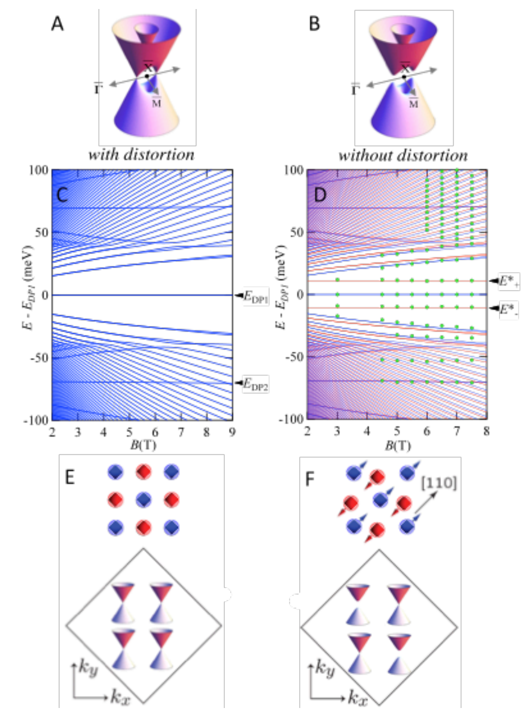

Figure 1: Coexistence of massless and massive Dirac Fermions. A and C show the schematic band structure and theoretical calculation of LL fan diagram without a symmetry breaking term added to the Hamiltonian. (B) also shows comparison with the data points obtained from experimental LL spectra with the theoretical band structure parameters adjusted to match the data. (C) and (D) show the schematic arrangement of surface atoms and band structure with, (C), and without, (D), a crystal

2. **Orbital texture of Dirac surfaces states probed by scanning tunneling spectroscopy.** Published in ***Nature Physics*** 10, 572–577 (2014)

A fundamental property predicted for the newly discovered topological crystalline insulator (TCI) family of materials is that due to symmetry constraints the orbital character of the surface state (SS) bands is different above and below the Dirac point. Both orbital- and spin-texture are therefore essential for a complete description of the TCI SS band structure. To experimentally probe this, we measured the interference patterns produced by the scattering of SS electrons of

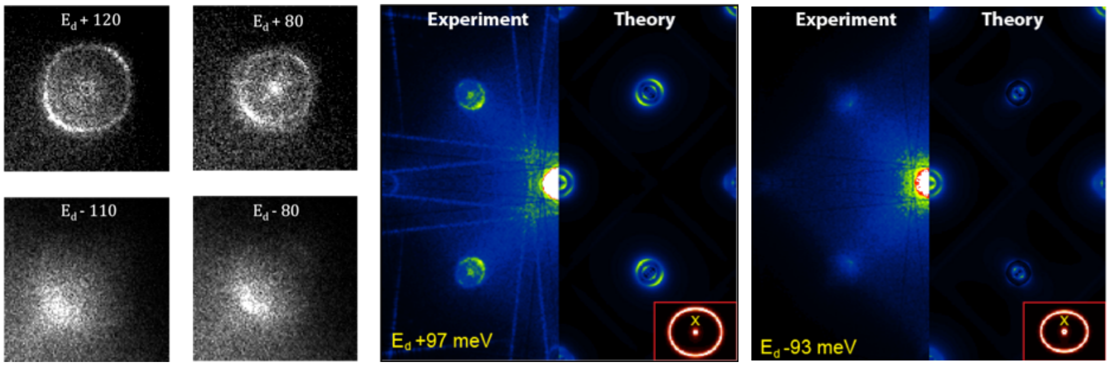

Figure 2 (Left) STM Fourier transforms above and below the Dirac point showing the effects of orbital depending scattering. (Middle and right) Comparison between STM data and theory.

$Pb_{1-x}Sn_xSe$ in the topological regime by scanning tunneling spectroscopy (STS). Fourier transforms (FTs) of the interference patterns show a marked change with energy across the Lifshitz transition. Importantly, we find that the intensity and energy dependence of the FTs show distinct characteristics, which by comparison with theory can be attributed to orbital effects (Fig. 2). Our results demonstrate the impact of orbital texture in scattering processes measured by STS and reveal the distinct orbital nature of the Dirac bands in this new class of topological materials.

3. **Phase transition in TCIs: Mass and surface state evolution from the topological to trivial phase.** Published in ***Nature Materials*** 14, 318–324 (2015)

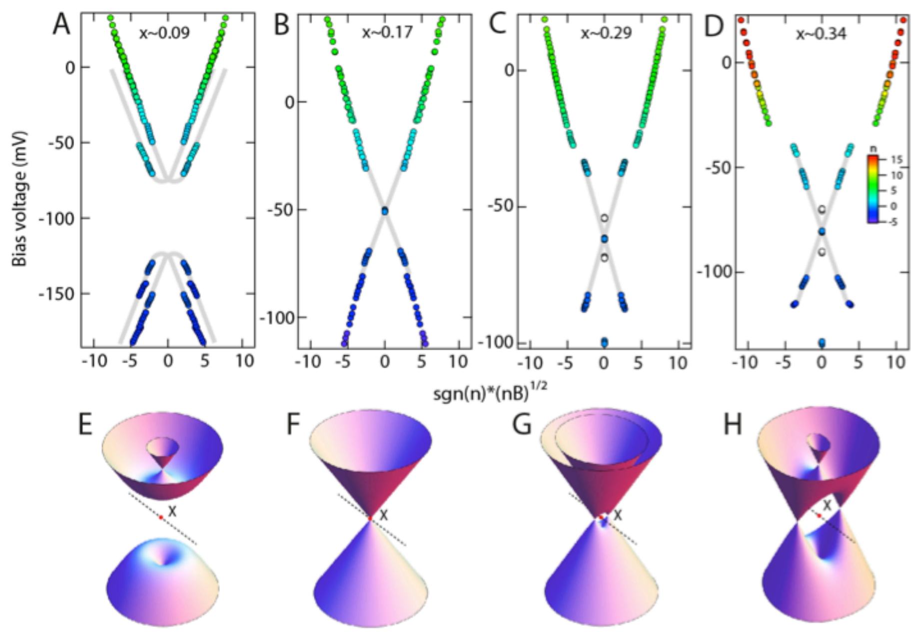

Figure 3. Landau level data showing the evolution of the Dirac surface states from the trivial to the topological regime. The schematic band structure from our data is shown below.

A central question in the field of topological insulators involves the fate of the Dirac surface states when band inversion is undone and the material becomes non-topological. The transition of topological surface states into the trivial phase has remained elusive in part due to lack of suitable materials. Here, we use scanning tunneling microscopy to track the quantum phase transition in a topological crystalline insulator (TCI), $Pb_{1-x}Sn_xSe$, tuned by Sn content. We discover the existence of surface states in the trivial phase that have the characteristics of gapped, double-branched Dirac fermions (Fig. 3). We demonstrate how these states induced by proximity to the topological phase, morph into robust topologically protected Dirac surface states across the critical composition. Our new theory for the non-topological SS indicates that this transformation is created by the reversal of Dirac fermion chirality, which naturally accompanies the topological phase transition in the bulk. Furthermore, we image the symmetry breaking distortion that leads to massive Dirac Fermions and track the evolution of the mass across the phase transition. Our results establish the highly tunable nature of TCIs with constantly evolving fermiology as a function of composition, which goes beyond topology and crystalline symmetries and shows unexpectedly rich behavior.

4. **Strain induced momentum space shift of Dirac node in heteroepitaxial thin films of SnTe/PbSe,** Published in ***Nature Nanotechnology*** 10, 849–853 (2015)

In TCIs the unique crystalline protection of the surface state (SS) band structure has led to a series of intriguing predictions of strain generated phenomena, from the appearance of pseudo-magnetic fields and helical flat bands, to the tunability of the Dirac SS by strain that may be used to construct `straintronic' nanoswitches. However, practical realization of this exotic phenomenology via strain engineering is experimentally challenging and is yet to be achieved. In this work, we have designed an experiment to not only generate and measure strain locally, but to also directly measure the resulting effects on the Dirac SS. Thin films of the TCI SnTe were grown insitu and measured by high-resolution scanning tunneling microscopy (STM). Heteroepitaxial thin films of SnTe host regions of both tensile and compressive strain. Large scale STM images were analyzed to reveal picoscale changes in the atomic positions in the strained regions and simultaneous Fourier-transform (FT) STM was used to determine the effects of strain on the Dirac electrons. We find that strain continuously tunes the momentum space position of the Dirac points. This is consistent with theoretical predictions and furthermore proves the fundamental mechanism necessary for using TCIs in a strain-based nanoswitches. This work establishes TCIs as a highly tunable platform for nanoscale quantum devices.

5. **Electron-phonon coupling probed by Landau level spectroscopy.** Published in ***Nature Communications*** 6, 6559 (2015)

Quantifying the interaction between phonons and electrons is of immense importance for a complete understanding of many materials systems. Nearly all information about electron-phonon coupling (EPC) is contained in the Eliashberg function of the material, but its precise extraction has in part been limited due to the lack of local experimental probes. By utilizing Landau level spectroscopy, we have constructed a method to directly extract the Eliashberg function, and demonstrate its applicability to lightly doped thermoelectric bulk insulator PbSe[3]. In addition to its high energy resolution only limited by thermal broadening, as well as access to both occupied and unoccupied electronic states, this novel experimental method could be used to detect variations in mass enhancement factor (λ) on microscopic length scales, which opens up a unique pathway for investigating the effects of chemical defects, surface doping and strain on λ.

6. **Nanoscale measurements of the strain tensor and its effects on local electronic properties** (to be submitted) We study the influence of the orbital nature of bands on their stain response. Orbital degrees of freedom have strong effects on the fundamental properties of electrons in solids. In addition to influencing bandwidths, gaps, correlation strength, and dispersion, orbital effects have also been implicated in generating novel electronic and structural phases such as Jahn-Teller effect and colossal magneto resistance. Here we show for the first time how the orbital nature of bands can create non-trivial strain effects. We use scanning tunneling microscopy (STM) to study the influence of strain on the electronic structure of a heteroepitaxial thin film of a topological crystalline insulator, SnTe. First we demonstrate how the complete strain tensor can be directly measured on the local scale with nanometer precision using STM. This allows us to create two-dimensional maps of biaxial, uniaxial and sheer strain components (Fig. 4), which can then be correlated with the local electronic structure using local Fourier-transform scanning tunneling spectroscopy. Applying these techniques to SnTe thin films, we find a surprising effect where uniaxial strain in one direction affects the band structure in the

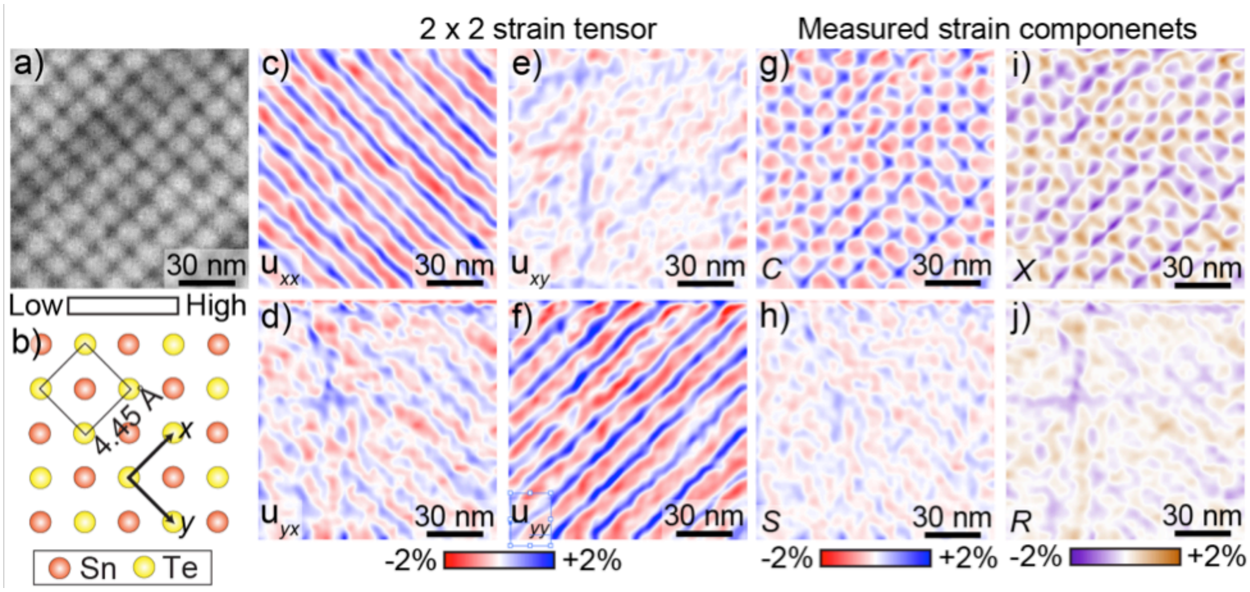

Fig. 4 Spatial distribution of different types of strain. (a) STM topograph of ~130 nm square region of the sample (V_{set} = -50 mV, I_{set} = 200 pA) (b) Schematic of the (001) surface of SnTe. Arrows in (b) denote the x- and y-axes. (c)-(f) The components of the 2 x 2 strain tensor extracted from topograph in (a). u_{ij} denotes . (g)-(j) Physically significant linear combinations of the tensor elements in (c)-(f): (g) The isotropic compression ; (i) the uniaxial strain ; (h) the shear strain ; (j) the local rotation angle .

perpendicular direction. Theoretical calculations indicate that this arises from the effects of strain on hopping matrix elements, which depend on the orbital quantum number of the bands. Our results imply that a microscopic model capturing strain effects on band structure must include a consideration of the orbital nature of the bands.

Publications

1. Daniel Walkup, Ilija Zeljkovic, Badih Assaf, Kane L Scipioni, R. Sankar, Fangcheng Chou and **Vidya Madhavan** Nanoscale measurements of the strain tensor and its effects on local electronic properties, (in preparation, 2016)

2. Ilija Zeljkovic, Daniel Walkup, Badih Assaf, Kane L Scipioni, R. Sankar, Fangcheng Chou, **Vidya Madhavan*,*** Strain engineering Dirac surface states in heteroepitaxial topological crystalline insulator thin films, ***Nature Nanotechnology*** 10, 849–853 (2015)

3. Ilija Zeljkovic, Kane L Scipioni, Daniel Walkup, Yoshinori Okada, Wenwen Zhou, R. Sankar, Guoqing Chang, Yung Jui Wang, Hsin Lin, Arun Bansil, Fangcheng Chou, Ziqiang Wang and **Vidya Madhavan**, Nanoscale Determination of the Mass Enhancement Factor in the Lightly-Doped Bulk Insulator Lead Selenide, ***Nature Communications*** 6, 6559 (2015)

4. Ilija Zeljkovic, Yoshinori Okada, Maksym Serbyn, R. Sankar, Daniel Walkup, Wenwen Zhou, Junwei Liu, G.Chang, Yung Jui Wang, M. Zahid Hasan, Fangcheng Chou, Hsin Lin, A. Bansil, Liang Fu and **V. Madhavan**, Dirac mass generation from crystal symmetry breaking on the surfaces of topological crystalline insulators, ***Nature Materials*** 14, 318–324 (2015)

5. Ilija Zeljkovic, Yoshinori Okada, Cheng-Yi Huang, R. Sankar, Daniel Walkup, Wenwen Zhou, Maksym Serbyn, Fangcheng Chou, Wei-Feng Tsai, Hsin Lin, A. Bansil, Liang Fu, M. Zahid Hasan and **V. Madhavan,** Mapping the unconventional orbital texture in topological crystalline insulators, ***Nature Physics*** 10, 572–577 (2014)

6. Yoshinori Okada, Maksym Serbyn, H. Lin, Daniel Walkup, W. Zhou, C. Dhital, Madhab Neupane, Suyang Xu, Yung Jui Wang, R. Sankar, F. Chou, Arun Bansil, M. Zahid Hasan, Stephen D. Wilson, Liang Fu and **V. Madhavan**, Observation of Dirac node formation and mass acquisition in a topological crystalline insulator, ***Science*** 341***,*** *1496-1499* (2013)