Experimental Realization of a Topological Crystalline Insulator in SnTe

Topological insulators are a novel quantum state of matter where an insulating bulk hosts unusual gapless metallic states protected by time-reversal symmetry (TRS). Their discovery stimulated the search for new topological states protected by other symmetries, and a recent theory predicted the existence of "topological crystalline insulators" (TCIs) in which the surface states are protected by mirror symmetry of the crystal. We have performed angle-resolved photoemission spectroscopy (ARPES) of narrow-gap IV-VI semiconductor tin telluride (SnTe) and show the first experimental evidence for the TCI phase in this material. Our ARPES result clearly demonstrates a signature of double Dirac-cone surface states, distinctly different from so-far discovered topological insulators, opening new avenues for exotic topological phenomena.

The surface state of three-dimensional topological insulators is characterized by a Dirac-cone energy dispersion protected by TRS. In topological insulators, the TRS plays a key role in characterizing the topological properties such as the quantum spin Hall effect and the magnetoelectric effect [1, 2]. In contrast, in TCIs, metallic surface states are protected by mirror symmetry of the crystal [3]. It was recently shown theoretically by Hsieh *et al.* [4] that the TCI phase is realized in an insulating crystal having the rocksalt structure when a band inversion occurs at the high-symmetry L points of the bulk Brillouin zone. They also predicted that IV-VI semiconductor SnTe is such a TCI, while the isostructural PbTe is not. It is thus of particular importance to experimentally examine the possibility of the TCI phase in these semiconductors, in order to establish the concept of this new topological state of matter and possibly to find novel topological phenomena beyond the framework of known topological materials.

To elucidate the electronic states of SnTe, we have performed high-resolution ARPES experiments at BL-28A and Tohoku University [5, 6].

Figure 1(a) shows the ARPES intensity of SnTe in the valence-band region plotted as a function of wave vector and binding energy, measured for the {001} surface along the $\bar{\Gamma}\bar{X}$ high-symmetry line in the surface Brillouin zone as shown in Fig. 1(b). The $\bar{X}$ point of the surface Brillouin zone corresponds to a projection of the L point of the bulk Brillouin zone where a direct bulk-band gap resides and the appearance of topological surface states is predicted [4]. Our ARPES data clearly demonstrate that the bulk-band maximum is indeed located around the $\bar{X}$ point. As shown in Fig. 1(c), the ARPES intensity at the Fermi level (E_F) measured with the photon energy $h\nu$ = 21.2 eV exhibits a bright intensity pattern centered around the $\bar{X}$ point and is elongated along the $\bar{\Gamma}\bar{X}$ direction. The near-E_F band dispersion along the $\bar{\Gamma}\bar{X}$ cut [Fig. 1(d)] exhibits two sets

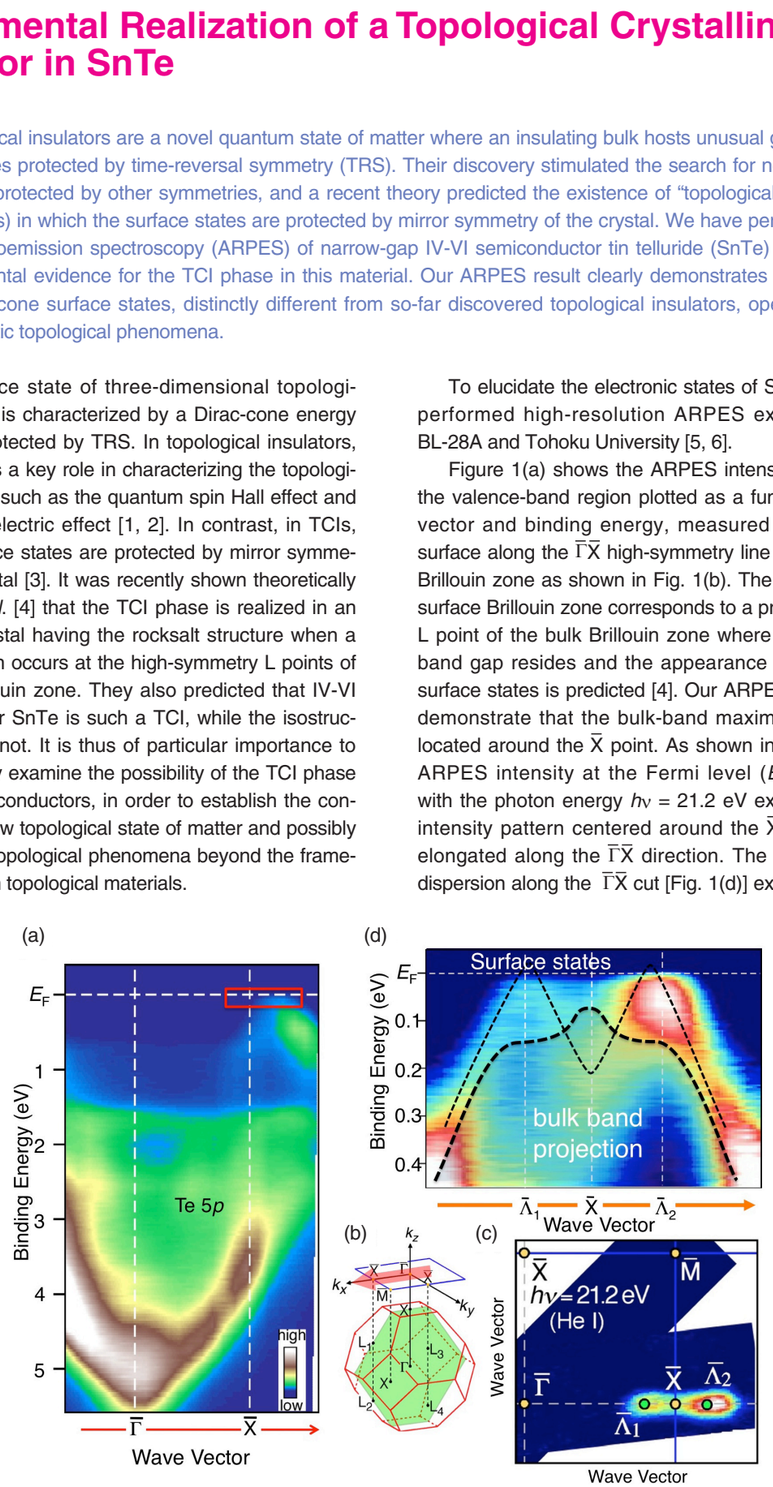

Figure 1: (a) Valence-band ARPES intensity of SnTe measured along the $\bar{\Gamma}\bar{X}$ cut. The red rectangle indicates the region where Dirac-cone dispersion exists. (b) Surface and bulk Brillouin zones of SnTe. (c) Fermi-surface mapping of SnTe. (d) Near-E_F band dispersion along the $\bar{\Gamma}\bar{X}$ cut.

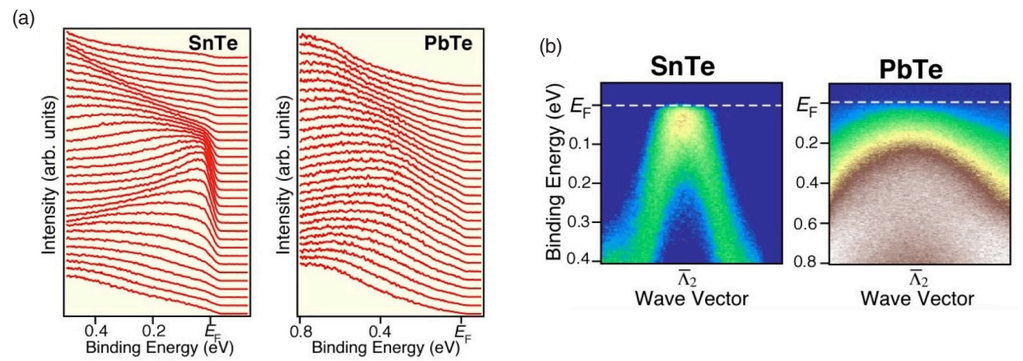

Figure 2: (a) Near-E_F ARPES spectra around the Dirac point (the $\bar{\Lambda}$ point) for SnTe and PbTe. (b) Corresponding ARPES-intensity plots.

of linearly dispersive bands crossing E_F, and the top of this Dirac-like band is located not at the $\bar{X}$ point but at a point slightly away from it (called here the $\bar{\Lambda}$ point). Such a characteristic "M"-shaped dispersion is not expected from the bulk-band calculations as can be seen from the plot of the bulk band projection [4] in Fig. 1(d), indicating that the observed Dirac-cone-like band originates from the surface states. The surface origin of the Dirac-cone band has also been confirmed by photon-energy dependent ARPES measurements where the Dirac-cone band shows negligible energy dispersion along the momentum perpendicular to the surface.

To clarify the uniqueness of SnTe among isostructural IV-VI semiconductors, we performed ARPES measurements of PbTe and directly compared the near-E_F electronic states around the Dirac point, as shown in Figs. 2(a) and (b). Intriguingly, the spectral feature of PbTe shows no evidence of the metallic Dirac-cone band, and displays only a broad feature originating from the top of the bulk valence band, suggesting that this material is an ordinary (trivial) insulator. This naturally suggests that a topological phase transition takes place in the solid-solution system $Pb_{1-x}Sn_xTe$ [6]. One can thus infer that the bulk-band gap closes at a critical x value, x_c, accompanied by a parity change of the valence-band wave function and an emergence/disappearance of the Dirac-cone surface state. Therefore, the present results have established for the first time the TCI phase in SnTe, which is in contrast to the trivial nature of isostructural PbTe. Our results unambiguously demonstrate the validity of the concept of TCI and suggest the existence of many more kinds of topological materials.

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