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Angle-resolved photoemission study of topological crystalline insulator $Pb_{1-x}Sn_xTe$

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1 Introduction

The discovery of topological insulators (TIs) triggered the search for new types of topological materials, and a recent theory predicted the existence of "topological crystalline insulators" (TCIs) in which metallic surface states are protected by point-group symmetry of the crystal structure. Such a TCI phase has been experimentally verified by angle-resolved photoemission spectroscopy (ARPES) experiments for narrow-gap IV-VI semiconductors SnTe [1], $Pb_{0.6}Sn_{0.4}Te$ [2], and $Pb_{0.77}Sn_{0.23}Se$ [3]. In those materials, the topological surface states measured on the (001) surface consist of double Dirac cones located at momenta slightly away from $\bar{X}$ point in the (110) mirror plane of the crystal. Since there are four $\bar{X}$ points on the boundary of the first surface Brillouin zone (BZ), there are a total of four Dirac cones within it. This is distinct from the three-dimensional (3D) TIs whose surface states are characterized by an odd number of Dirac cones. In contrast to the double Dirac-cone signature observed in the TCI phase, the ARPES measurements for isostructual PbTe [1] and $Pb_{0.8}Sn_{0.2}Te$ [2] revealed the absence of any surface states, which strongly suggests a trivial-to-nontrivial topological quantum phase transition (QPT) in the solid-solution system $Pb_{1-x}Sn_xTe$. We have performed comprehensive ARPES studies of $Pb_{1-x}Sn_xTe$ with various Sn compositions (x = 0.0, 0.2, 0.3, 0.5, 0.6, 0.8, and 1.0) to clarify how the surface and bulk electronic states evolve as a function of Sn composition x, which would be useful for establishing practical understanding of TCIs [4].

2 Experiment

High-quality single crystals of the two end-member samples SnTe (x = 1.0) and PbTe (x = 0.0) were grown by the modified Bridgeman method, and the solid-solution samples (x = 0.2, 0.3, 0.5, 0.6, and 0.8) were prepared by a vapor transport method. ARPES measurements were performed with a VG-Scienta SES2002 electron analyzer with a tunable synchrotron light at the beamline BL28A at Photon Factory (KEK). We used circularly polarized light of 75-100 eV. The energy and angular resolutions were set at 10-30 meV and 0.2°, respectively.

3 Results and Discussion

Figures 3(a) and (b) show the near-E_F ARPES intensity and corresponding EDCs, respectively, taken at hν = 78.5 eV. From photon energy dependence (75-100 eV), we have elucidated that hν ~78.5 eV hits to the right k_z value to probe the L point of the bulk BZ projected to the $\bar{X}$ point of the surface BZ. To elucidate the evolution of the surface states and bulk VB as a function of x, we have measured all the samples with hν = 78.5 eV along the k cut to cross the bulk VB top. At x = 1.0, we observe a highly dispersive holelike band which is attributed to an admixture of bulk and surface bands with dominant contribution from the surface state near E_F. As clearly seen, the holelike band still touches to the E_F at x = 0.3, suggesting the existence of metallic surface state. However, at x = 0.2 the holelike band is obviously away from E_F, indicating the surface state vanishes at $x_c \approx 0.25$. From the x dependence of the energy location of VB maximum (not shown), we also found that VB maximum approaches E_F as x is reduced from 1.0 toward x_c, and then it moves away from E_F when x passes x_c, suggesting the band inversion at x_c. With this band inversion, we conclude that the phase transition at $x_c \approx 0.25$ is indeed of topological origin, separating the TCI and trivial phase.

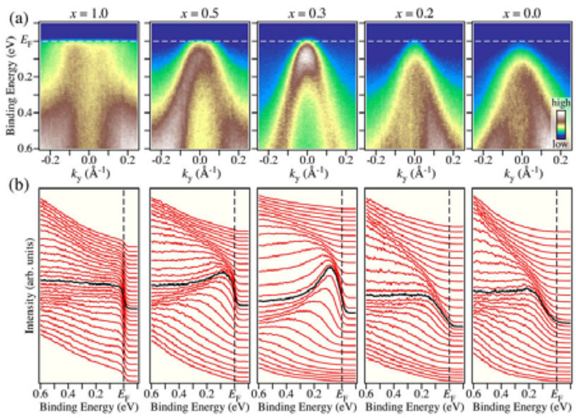

Fig. 1: (a), (b) x dependence of near-E_F ARPES intensity and corresponding EDCs, respectively, measured along the k_y cut across the bulk VB top that can be accessed with hν = 78.5 eV.

References

[1] Y. Tanaka *et al*., *Nature Phys.* **8**, 800 (2012).
[2] S.-Y. Xu, *et al*., *Nature Commun*. **3**, 1192 (2012).
[3] P. Dziawa *et al*., *Nature Mat*. **11**, 1023 (2012).
[4] Y. Tanaka *et al*., *Phys. Rev. B* **87**, 155105 (2013).

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