Angle-resolved photoemission study of topological crystalline insulator Pb$_{1-x}$Sn$_x$Te

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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 isostructural PbTe [1] and Pb$_{0.6}$Sn$_{0.4}$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$_x$Te. We have performed comprehensive ARPES studies of Pb$_{1-x}$Sn$_x$Te with various Sn compositions ($x = 0.0, 0.2, 0.3, 0.5, 0.6, 0.8, 1.0$) 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 ($x = 0.2, 0.3, 0.5, 0.6, 0.8$) 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 $h\nu = 78.5$ eV. From photon energy dependence (75-100 eV), we have elucidated that $h\nu \sim 78.5$ eV hits to the right $k$ 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 $h\nu = 78.5$ 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 $x = 0.25$. 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 $x_c = 0.25$ is indeed of topological origin, separating the TCI and trivial phase.

References


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