Core-level photoemission study of $TlBiSe_2$ (111) surface

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Introduction

Topological insulator is currently a hot topic in condensed matter physics. On surfaces of topological insulators, spin-polarized surface states appear in bulk band gap and disperse as massless Dirac Fermions. The characteristic spin and electronic structure of such surface states derives novel transport phenomena such as the spin-Hall effect. In principle, surface states on a topological insulator are dependent on bulk electronic structure and the surface states are robust with respect to nonmagnetic defects and disorder. On the other hand, according to the theoretical works [1,2], termination, surface relaxation and surface reconstruction is closely related to the surface electronic structure.

Ternary chalcogenide $TlBiSe_2$ is known to be one of three-dimensional topological insulators. The crystal structure is characterized by the stacking sequence of -Se-Bi-Se-Tl-Se- along the [111] direction. The Dirac-cone surface state in the bulk band gap of 0.35 eV was observed for the cleaved (111) surface [3,4]. Because the bulk band gap is substantially larger than the thermal energy at room temperature, $TlBiSe_2$ is expected to be a key material for practical application of topological insulators. However, as far as we know, the structure of the cleaved $TlBiSe_2$ (111) surface has not yet clarified. In order to study the atomic structure of this surface, we performed photoelectron spectroscopy (PES) measurements of the core levels of Tl 5d, Bi 5d and Se 4d.

Experiment

The photoemission experiments were performed at KEK-PF BL-18A. We used a SES100 spectrometer to measure valence band mapping in an angle-resolve PES (ARPES) mode and wide-range core-level spectra in the normal emission, and an ADES-500 spectrometer to obtain the emission-angle and photon-energy dependence of the core levels with a fixed incident angle of 45°. The photon energy used in core-level PES ranges from 50 to 130 eV. These PES measurements were performed at room temperature.

A $TlBiSe_2$ crystal was grown by the Bridgeman method. The orientation of a sample wafer was determined by X-ray diffraction to be (111). The sample was cleaved at pressure below 1×10^{-7} Torr in the preparation chamber and immediately transferred to the analyzer chamber at 2×10^{-10} Torr. Low-energy electron diffraction (LEED) showed a sharp (1×1) pattern as shown in Fig. 1(a). The three-fold symmetry of the LEED pattern is clearly seen.

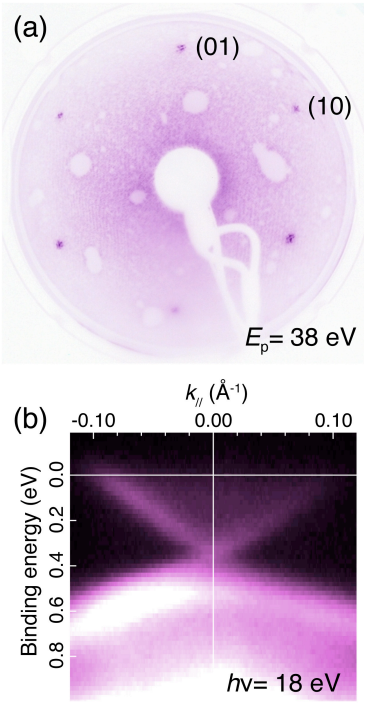

Fig. 1: (a) LEED pattern of the $TlBiSe_2$ (111) surface at room temperature. (b) An ARPES band mapping near the Fermi level along $\bar{\Gamma}\bar{K}$.

Results and discussion

Figure 1(b) shows an ARPES band mapping near the Fermi level (E_F). The characteristic dispersion of the Dirac-cone surface state is seen around 0.3 eV below E_F. The cross point appears at 0.35 eV below E_F, which is ~50 meV higher than that reported in the previous studies [3,4]. The difference is probably due to slight misalignment. From the ARPES band mapping, it is confirmed that we obtained a clean $TlBiSe_2$ (111) surface.

The normal-emission core-level spectra with 90-eV photons is shown in Fig. 2(a). In contrast to sharp Bi and Se peaks, the Tl 5d peaks have double components. The center of the lower-binding-energy component, labeled α, is located at 12.8 eV. The energy difference between the higher-binding-energy component, labeled β, and α is evaluated to be 0.4 eV. The width of both peaks is ~0.28 eV, which is almost same as the Bi 5d and Se 4d peaks. We observed that the relative intensity of the component α decreases with decreasing photon energy. The intensities of the two components were comparable in the normal emission specrum with $h\nu$=70 eV. It is noted that a similar sattelite structure of Tl 5d core-level is reported for $TlBiTe_2$ [5], which also has a Dirac-cone surface state while the bulk electronic structure is semimetallic.

In bulk crystal of $TlBiSe_2$, the interlayer distance between Tl and Se layers is larger than that between Bi and Se, indicating the relatively weak bond between Tl-Se. Thus Tl or Se termination is expected to appear on the cleaved surface. However, one cannot know which termination is exposed when a crystal is cleaved. On the other hand, it is reported in the theoretical work [1] that both the surface models with Tl and Se termination do not reproduce the observed surface-state band dispersions. In order to resolve this problem for the $TlBiSe_2$ (111) surface, the precise structure analysis by diffraction methods is required.

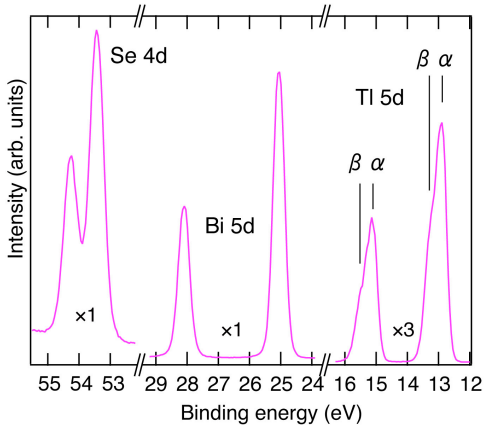

Fig. 2 Normal-emission core-level spectra of the cleaved $TlBiSe_2$ surface with $h\nu$=90 eV.

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