

ARPES study of high ZT thermoelectric material SnSe

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1 Introduction

Thermoelectric materials enable direct conversion between temperature difference and electric current, and can be used to produce electric power from waste heat. Therefore finding a new thermoelectric material is one of the important routes to solve energy problem. The performance is evaluated with the dimensionless figure of merit, $ZT = S^2\sigma/\kappa$, where T , σ , and κ are Seebeck coefficient, absolute temperature, electric, and thermal conductivity, respectively.

In this study, we have performed angle-resolved photoemission spectroscopy (ARPES) experiments on high ZT SnSe [1] in order to determine the band dispersions of the top of the valence band experimentally. Synchrotron based ARPES is capable of determining the electronic band structure in the whole momentum space. We found that though experimentally observed whole valence band structure is similar to calculated ones [2], it shows some deviation from the calculation.

2 Experiment

SnSe single crystals were provided by Takano's group, NIMS. ARPES measurements on were performed at BL-28A of Photon Factory with circularly polarized light. All the data were taken with a Scienta SES2002 electron analyzer, with the energy resolution set to 20 meV. The samples were cleaved *in situ* in a-plane (parallel to Γ ZTY plane) at 20 K and under the base pressure of better than 1.7×10^{-8} Pa. The samples were kept under the same condition during measurements. No change of the spectral shape was observed during the measurement.

3 Results and Discussion

Figures 1(b) and 1(c) show the valence band ARPES intensity maps of SnSe measured along the c^* direction in the bulk Brillouin zone (BZ) (Fig. 1(d)) with photon energy of 72 eV and 80 eV, respectively, together with calculated band dispersions (Kuroki's group, Osaka Univ.) along corresponding high symmetry directions in BZ. In both figures, experimental band dispersions, which appear as bright regions, disperse symmetric with Γ (X). The top of the valence band is located near the Fermi level (E_F) and at slightly away from Z. Since the band gap of SnSe at room temperature is reported to be 0.86-0.898 eV, the location of the valence band top near E_F indicates that p-type nature of the sample. Several bands closely

located between E_F and 4 eV binding energy are seen, which are derived from mainly Se 4p orbitals hybridized with Sn 5s,p orbitals. We also found a separate band having a top around Γ (X) and its bottom around Z(U) in the energy region from 5 to 8 eV, which is a dominant Sn 4p derived band. We found overall correspondence between experimental and calculated band dispersions, indicating that the band calculation can be a good guidance to understand the electronic structure of SnSe.

From the direct observation of band dispersions around the top of the valence band maxima, we determine their relative energy and effective masses of two hole bands [2], which are indispensable to understand the thermoelectric properties.

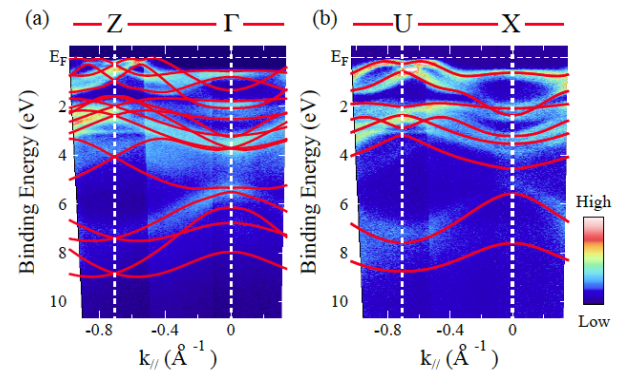


Fig. 1: The ARPES intensity plots of valence band parallel to c^* axis taken with photon energy of 72 eV and 80 eV, respectively, which are overlaid with calculated bands along Γ -Z and X-U lines [2].

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