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Angle-resolved Photoemission Spectroscopy Study on the Surface States of the Correlated Topological Insulator YbB_6

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1 Introduction

Rare earth borides possess a variety of interesting electronic and magnetic properties, including mixed valence, heavy fermion, and superconducting behaviors [1-4], and they have been under intensive studies for decades due to their potential application on spintronics [5], thermionic electron sources [6], etc. Recently, band structure calculations rekindled people's interests on SmB_6 as a possible candidate of the first topological Kondo insulator [7, 8]. Numerous experiments have been performed to seek for the topological surface states [9, 10]. However, the surface states can only exist in low temperature and the coexistence of the bulk bands and surface states in SmB_6 limits its future applications.

YbB_6 is another rare earth hexaborides which shares the same CsCl type crystal structure with SmB_6 [11], and is predicted to be a correlated topological insulator with a bulk insulating gap of about 31 meV [12]. The large bulk band gap makes this system practically important for applications based on topological surface states. However, despite the previous successes of density functional theory in predicting topological insulators [13, 14], significant electron correlation in rare earth compounds pose new challenges to theory and calculations. Understanding the electronic structures of these systems will more rely on the experiments. Among many other experimental methods, angle-resolved photoemission spectroscopy (ARPES) is still the most powerful tool to identify the electronic structure directly [10, 15], and help sort out the correlation effects on the novel topological states.

2 Experiment

High quality YbB_6 single crystals were synthesized by the Al-flux method. A chunk of Yb together with the powders of Boron and Al were mixed with a ratio of 1:6:400 and heated to 1,773 K in an alumina crucible in the argon atmosphere, then maintained at 1,773 K for about 2 days before slowly cooling down to 873K at 5K per hour. ARPES measurements were performed at beamline 28A of Photon Factory, KEK, equipped with a Scienta SES-2002 electron analyzer. The angular resolution was 0.2° and the overall energy resolution was 20meV or better depending on the photon energy. The samples were cleaved *in situ* along the (001) plane and measured under ultra-high vacuum below 3×10^{-8} Pa.

3 Results and Discussion

Fig. 1 (a) shows the photoemission intensities of YbB_6 over a large energy scale, the non-dispersive Yb 4*f* bands are located at 1eV and 2.3eV below E_F, identified in the integrated energy distribution curve (EDC). They correspond to the $^2F_{7/2}$ and $^2F_{5/2}$ multiplets of the Yb^{2+} $4f^{14}\rightarrow4f^{13}$ final states based on the LDA calculations [12]. The energy difference between the two multiplets is 1.3 eV, consistent with the calculation. However, the energy positions of these *4f* bands are deeper than that calculated in Ref. [12], suggesting correlation effects need to be reconsidered in calculation. In addition, some dispersive features are resolved in the low energy range, which may mostly originate from the Yb *5d* orbitals [12].

To search for the predicted surface states in YbB_6, the photoemission intensity map taken at E_F is shown in Fig. 1(b). Elliptical Fermi surfaces located around X are clearly observed. The nature of these states can be further revealed in their dispersions. Fig.1(c) illustrates the photoemission intensities near E_F along cut #1 and #2, from which we can clearly resolve linear dispersed bands around X. These bands cross at about -250meV below E_F, suggesting the position of a Dirac point (DP). However, the behavior of these bands below DP could not be resolved due to the strong residual intensity of the flat 4f bands. In addition, we have not resolved surface state as predicted around Γ, due to the weak intensity caused

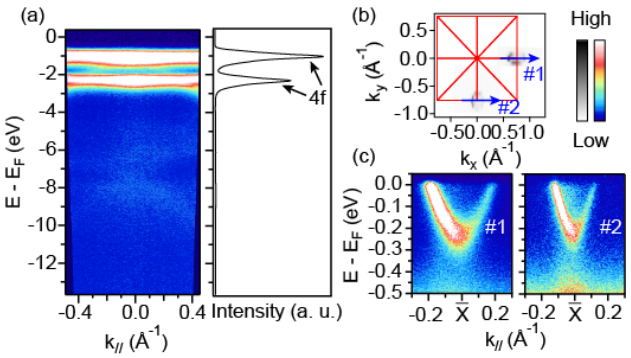

Fig.1 (a) Photoemission intensity plot and the corresponding EDC showing the valence band structure of YbB6. The flat 4f bands are marked by the arrows. (b) Photoemission intensity map at E_F taken with 70 eV photons. The intensity was integrated over a window of [E_F - 10meV, E_F + 10meV]. (c) The photoemission intensity plot along cut #1 and cut #2 measured with 70 eV photons.

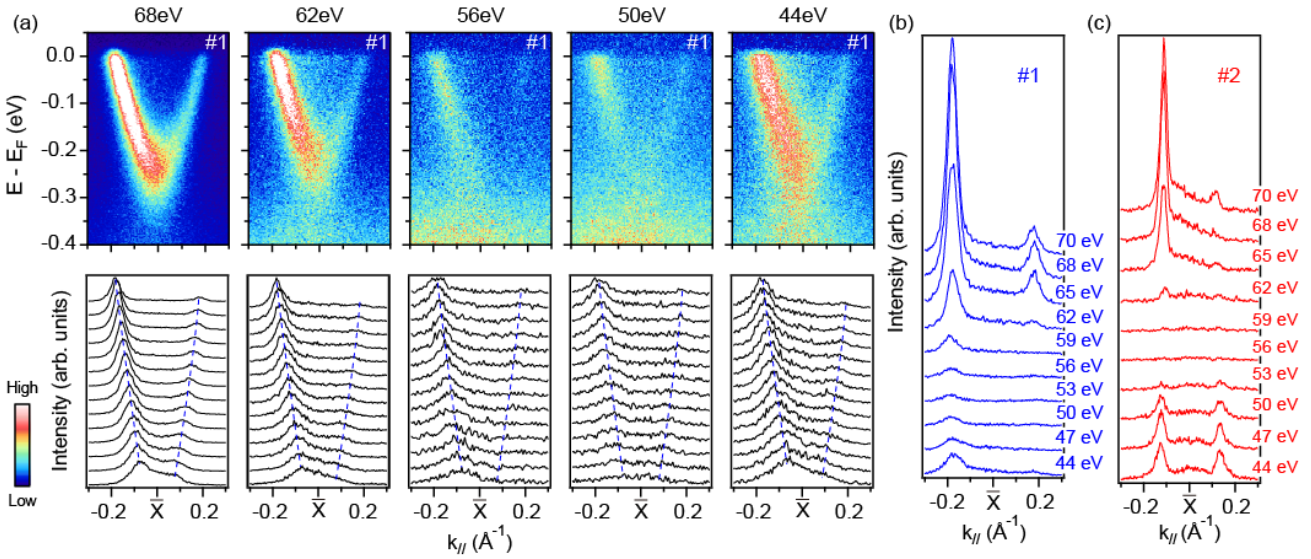

Fig. 2: (a) Photon energy dependence of the photoemission intensity measured along cut #1 and their corresponding MDC plots within [E_F -200meV, E_F]. (b) (c) The MDCs integrated within 20meV below E_F of each photo energy along cut #1 and cut #2.

by photoemission matrix element effect in this energy range.

To have a comprehensive understanding of the k_z evolution and confirm the surface origin of the low lying bands, we varied the photon energies to study their dispersion along k_z, as illustrated in Fig. 2. The photoemission intensity distribution along #1 direction taken with different photon energies are presented in Fig. 2(a). Clear *E-k* dispersions are observed in the photoemission intensity distributions, and they do not show any noticeable change with k_z. We extrapolate the dispersion of the bands from the momentum distribution curves (MDC) taken with 68eV photons and overlaid it on the data taken with other photon energies, which clearly show that the dispersions and Fermi crossings are k_z independent. Moreover, the MDCs at E_F along #1 and #2 shown in Fig. 2(b) and 2(c) also demonstrate their two-dimensional nature

Since topological surface states (TSS) resulted from spin-orbit interaction are formed by spin-nondegenerate Dirac fermions, a key feature of TSS is their spin chiral

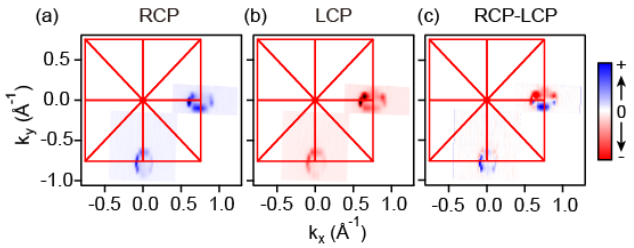

Fig. 3: (a) (b) Fermi surface maps of YbB_6 taken with right circularly polarized (RCP) and left circularly polarized (LCP) light, respectively. The intensity was integrated within 20meV at E_F. The data were taken at 15 K with 70 eV photons. (c) The intensity difference between the RCP and LCP Fermi surface maps in panels a and b.

structure [16]. Both the spin and orbital angular momentum (OAM) are interlocked and rotate with the electron momentum (*k*), so that the total angular momentum *J* is conserved. This provides the foundation to examine the spin polarity through the chirality of the OAM with the so-called circular dichroism (CD) of ARPES.

Comparing the Fermi surface maps measured under right-handed circular polarized (RCP) light and left-handed circular polarized (LCP) light shown in Figs. 3(a) and 3(b), we can clearly see the difference resulted from the polarizations. The intensity of the right electron pocket is higher on the lower side than that on the upper side for the RCP data, while the LCP data exhibit an opposite behavior. The lower electron pocket does not show clear switching of high intensity regions between the positive k_x side and negative k_x side with different circularly polarized light, thus we could not get a definite conclusion. The CD can be more clearly represented by the net difference RCP-LCP in Fig. 3 (c). The CD results do suggest that the chirality of OAM exists, indicating that they might possess helical spin textures, further support their topological origin.

For a surface state, the work function depends directly on the surface conditions. In addition to the band structures shown in previous figures, we also observed hole like pockets in YbB_6 as shown in Fig. 4 (a)-(c). To compare the different chemical potential, the integrated large scale EDCs are shown in Fig. 4 (d) to reveal the bulk 4*f* band position. Taking the Fermi level as reference, one sees the evolution of the surface states associated with the shift of Yb 4*f* band. With the upward shift of the Yb 4*f* band, the Dirac point also rises and is dramatically higher than E_F. SmB_6 is known as a Kondo insulator, but YbB_6 is not, which can be confirmed by the temperature dependence experiments. As the temperature rises from

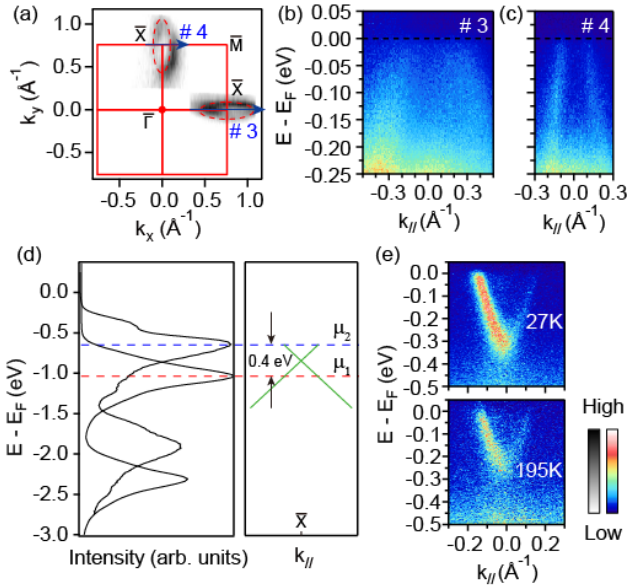

Fig. 4: (a) The photoemission intensity map of one sample showing hole like pockets and (b) (c) two cuts taken along cut #3 and #4. (d) A schematic plot to show the chemical potential shift in different surfaces and the integrated EDCs of the two samples to compare the different chemical potential. μ_1 and μ_2 refer to the chemical potential of the two sample. (e) The photoemission intensity data taken along cut #2 at 27K and 195K, respectively.

27K to 195K, the band structure shows no obvious change [Fig. 4 (e)].

To summarize, we have obtained a comprehensive understanding of the electronic structure of YbB_6, which has a much larger insulating gap than SmB_6. We directly observe several dispersive states within the insulating gap of YbB_6. These states show negligible k_z dependence, which indicates their surface origin. Moreover, we perform photoemission circular dichroism experiments, which suggest that the low energy states possess chirality of the orbital angular momentum. These states are sensitive to chemical potential and do not vanish at high temperature, which makes YbB_6 a more promising compound for application than SmB_6.

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Research Achievements

1. M. Xia, et al., Angle-resolved Photoemission Spectroscopy Study on the Surface States of the Correlated Topological Insulator YbB6, Preprint at http://arxiv.org/abs/1404.6217 (2014).

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