Topological Order of the Kondo Insulator SmB_6 Unveiled from a New Crystal Orientation

Recently, the non-trivial topological order of Kondo insulators has attracted much attention because of the expected collaboration effect on its topological surface electronic states with strong electron correlation. Here, we obtained a well-defined clean surface of SmB_6 facing a new crystal orientation, (111), with smaller numbers of time-reversal invariant momenta than those on the (001) cleaved plane and revealed its surface electronic structure by angle-resolved photoelectron spectroscopy. The obtained surface state indicated non-trivial topological order, which was not clear from the (001) surface, making SmB_6 a fertile playground to study the strongly correlated topological electronic states.

The topological order of crystals is known as a major origin for realizing exotic low-dimensional electronic structures, especially on the edge (surface) of the crystals [1]. Among them, materials in which the non-trivial topological order cooperates with strong electron correlation are expected to be a suitable field to study various unconventional electronic phenomena, such as the Kondo breakdown of the topological surface state (TSS) [2]. One of such strongly correlated topological materials is a topological Kondo insulator (TKI). TKI is based on a Kondo insulator with a very narrow bulk bandgap appearing at low temperatures due to the Kondo effect, and it has a non-trivial topological order resulting in TSS dispersing across the bulk Kondo gap [3]. Therefore, TKI is attracting much attention as a typical case of the coexistence of topological order and strong electron correlation.

Samarium hexaboride (SmB_6) has long been known as a Kondo insulator [4] with the Kondo gap and was one of the first materials to be proposed as a candidate of TKI from a theoretical calculation [3]. However, for experimental reasons, its topological order has been unclear for years because of the difficulty of interpreting the topology of the obtained surface electronic states from the (001) cleaved surface, which is the only crystal orientation obtained so far [5, 6]. The cause of this difficulty is the rather large number of surface time-reversal invariant momenta (TRIM) on the (001) surface [three, see Fig. 1(a)], and multiple surface terminations with surface reconstructions there. In this work, we observed the surface electronic structure of single-crystal SmB_6 from the (111) surface for the first time, in order to elucidate its topological order. Since the number of surface TRIMs on the (111) surface is expected to be minimum [two, as shown in Fig. 1(a)], we chose this orientation to determine the topological order of SmB_6 in a simple manner.

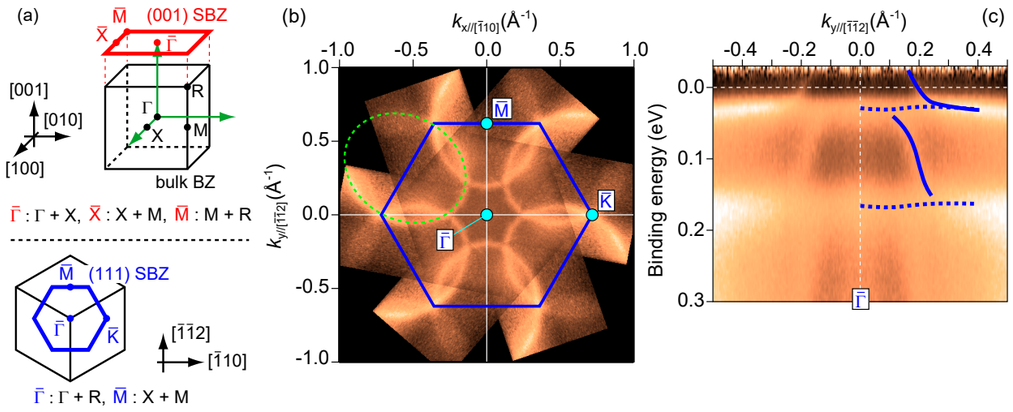

Figure 1: (a) Surface and bulk Brillouin zones (BZ) of SmB_6 along (001) and (111) surface orientations. **(b)** Fermi contour of the SmB_6(111) surface obtained by ARPES at 15 K ($h\nu$ = 35 eV, circularly polarized photons), symmetrized based on the three-fold rotation and time-reversal symmetry. The hexagon is the surface BZ boundary. The dashed oval guides the shape of a surface Fermi contour. **(c)** Band dispersion of the SmB_6(111) surface obtained by ARPES [the same condition as (b)] taken along [-1-12]. ARPES intensities are divided by the Fermi distribution function convolved with the instrumental resolution. Figures are from the same data as ref. [7].

The single crystals of SmB_6 grown by the floating-zone method were mechanically polished in air until a mirror-like shiny surface was obtained. Then, the polished sample was heated in an ultra-high vacuum chamber up to ~1700 K for 15 min. After heating, a sharp low-energy electron diffraction pattern as well as distinct band dispersions could be seen by angle-resolved photoelectron spectroscopy (ARPES) as shown in Figs. 1(b-c). ARPES measurements were mainly performed at BL-2A MUSASHI (proposal numbers: 2015G540 and 2017G537). The photon energy used in this work ranged from 35 to 80 eV and the energy resolution was estimated to be ~15 meV from a Ta foil attached to the sample.

Figure 1(b) is the Fermi contour obtained by ARPES. It clearly shows the contours surrounding the *M* points of the surface Brillouin zone (SBZ), as guided by the dashed oval. Around the Fermi level, no other electronic states were obtained by ARPES, indicating that these ovals are the unique metallic electronic structure of SmB_6(111) at 15 K. Since it is well known that the bulk electronic structure of SmB_6 is insulating, these Fermi contours should be derived from the surface. Indeed, we found no k_z dispersion of the metallic states by sweeping the incident photon energies, indicating its two-dimensional nature consistent with the origin from the surface. Moreover, from the band dispersion shown in Fig. 1(c), the surface Fermi contour is made by the continuous band dispersing across the Fermi level and merging into the nearly localized 4*f* band lying slightly below the Fermi level. Such behavior agrees well with what is expected for TSS. Combined with the lift of spin degeneracy in the surface band confirmed by spin-resolved ARPES performed elsewhere, the non-trivial topological order of SmB_6 is revealed from the newly obtained (111) clean surface.

This result makes SmB_6 an exciting material to study the collaboration effect between the topological order and strong electron correlation. Further studies, such as to clarify the origin of the inconsistent topological assignments obtained on SmB_6(001) and the temperature-dependent evolution of the TSS, which is expected to be influenced by the electron correlation, are ongoing.

REFERENCES

[1] M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045 (2010).
[2] C. Alexandrov, P. Coleman and O. Erten, *Phys. Rev. Lett.* **114**, 177202 (2015).
[3] M. Dzero, K. Sun, V. Galitski and P. Coleman, *Phys. Rev. Lett.* **104**, 106408 (2010).
[4] R. L. Cohen, M. Eibschütz, K. W. West and E. Buehler, *J. Appl. Phys.* **41**, 898 (1970).
[5] N. Xu X. Shi, P. K. Biswas, C. E. Matt, R. S. Dhaka, Y. Huang, N. C. Plumb, M. Radović, J. H. Dil, E. Pomjakushina, K. Conder, A. Amato, Z. Salman, D. McK. Paul, J. Mesot, H. Ding and M. Shi, *Phys. Rev. B* **88**, 121102 (2013).
[6] P. Hlawenka, K. Siemensmeyer, E. Weschke, A. Varykhalov, J. Sánchez-Barriga, N.Y. Shitsevalova, A.V. Dukhnenko, V.B. Filipov, S. Gabáni, K. Flachbart, O. Rader and E.D.L. Rienks, *Nature Commun.* **9**, 517 (2018).
[7] Y. Ohtsubo, Y. Yamashita, K. Hagiwara, S. Ideta, K. Tanaka, R. Yukawa, K. Horiba, H. Kumigashira, K. Miyamoto, T. Okuda, W. Hirano, F. Iga and S. Kimura, *Nature Commun.* **10**, 2298 (2019).

BEAMLINE

BL-2A

Y. Ohtsubo[1], Y. Yamashita[1], K. Hagiwara[1], R. Yukawa[2], K. Horiba[2], H. Kumigashira[2], W. Hirano[3], F. Iga[3] and S. Kimura[1] ([1]Osaka Univ., [2]KEK-IMSS-PF, [3]Ibaraki Univ.)