Nodal-line fermions protected by nonsymmorphic symmetry in Ta₃SiTe₆

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1 Introduction

The search for new types of topological materials hosting nodal fermions is currently one of emergent topics in condensed-matter physics. Recently, it was theoretically proposed that layered ternary telluride Ta₃SiTe₆ hosts the nodal fermions protected by the nonsymmorphic glide mirror symmetry [1]. This material crystalizes in the orthorhombic structure [Fig. 1(a)] with the space group No. 62 (Pnma). First-principles band-structure calculations show that, when the spin-orbit coupling (SOC) is neglected, Ta₃SiTe₆ displays a four-fold-degenerate (eight-folddegenerate if counting spin) nodal line on the SR line in the bulk Brillouin zone (BZ) shown in Fig. 1(b) due to the band crossing protected by the glide mirror symmetry. It is also suggested that when the SOC is included, the four-fold degeneracy on the SR line is slightly lifted and as a result the hourglass-like dispersions appear in the close vicinity of $E_{\rm F}$. To examine such intriguing predictions, it is highly desirable to experimentally establish the electronic band structure of Ta₃SiTe₆.

2 Experiment

High-quality single crystals of Ta₃SiTe₆ were grown by the chemical vapor transport method by using I₂ as Angle-resolved photoemission transport agent. spectroscopy (ARPES) measurements were performed with a DA30 electron analyzer at BL28. To excite photoelectrons, we used linearly polarized VUV light of 40-100 eV. The energy and angular resolutions were set to be 6-20 meV and 0.2°, respectively. We also measured the core-level spectrum with 600-eV photons at BL2. Crystals were cleaved *in-situ* along the (001) plane in an ultrahigh vacuum of 1×10⁻¹⁰ Torr and showed a shiny mirror-like surface indicative of high quality of the crystal. Sample temperature during measurements was kept at T = 30 K.

3 Results and Discussion

We show in Fig. 1(c) the ARPES-intensity mapping at $E_{\rm F}$ as a function of in-plane wave vectors (k_x and k_y) [2]. We observe two types of Fermi surfaces, one is an open Fermi surface with a holelike character, surrounding the $\overline{\Gamma}$ and $\overline{\rm Y}$ points with strong wiggling along the k_x direction. Another Fermi surface encloses the $\overline{\rm M}$ and $\overline{\rm X}$ points,

forming an open Fermi surface with an electronlike character. By utilizing the energy-tunable photons from synchrotron radiation, as shown in the normal-emission spectra in Fig. 1(d), we have determined the band structure in the 3D BZ, and found that the energy bands in the valence-band show Dirac-like dispersions which present a band degeneracy at the R point of the bulk orthorhombic Brillouin zone (not shown). This band degeneracy extends one-dimensionally along the whole SR high-symmetry line, forming the nodal lines protected by the glide mirror symmetry of the crystal. Our result thus suggests that the glide symmetry is highly useful to search for new platform of topological semimetals hosting nodal lines.



Fig. 1: (a) Crystal structure and (b) BZ of Ta₃SiTe₆. (c) ARPES intensity at E_F plotted as a function of k_x and k_y . (d) Plot of normal-emission ARPES intensity as a function of k_z [2].

References

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