Nodal-line fermions protected by nonsymmorphic symmetry in \( \text{Ta}_3\text{SiTe}_6 \)

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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 \( \text{Ta}_3\text{SiTe}_6 \) hosts the nodal fermions protected by the nonsymmetric glide mirror symmetry \(^1\). This material crystallizes in the orthorhombic structure \([\text{Fig. 1(a)}]\) with the space group No. 62 \((\text{Pnma})\). First-principles band-structure calculations show that, when the spin-orbit coupling (SOC) is neglected, \( \text{Ta}_3\text{SiTe}_6 \) displays a four-fold-degenerate (eight-fold-degenerate 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 \( E_F \). To examine such intriguing predictions, it is highly desirable to experimentally establish the electronic band structure of \( \text{Ta}_3\text{SiTe}_6 \).

2 Experiment
High-quality single crystals of \( \text{Ta}_3\text{SiTe}_6 \) were grown by the chemical vapor transport method by using \( \text{I}_2 \) as transport agent. Angle-resolved photomission 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 \( 1\times10^{-10} \) 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 \( E_F \) 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 hololike character, surrounding the \( \Gamma \) and \( \bar{Y} \) points with strong wiggling along the \( k_z \) direction. Another Fermi surface encloses the M and 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 \( \text{Ta}_3\text{SiTe}_6 \). (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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