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Dirac-nodal-arc surface state in the nodal-line semimetal HfSiS

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1 Introduction

The discovery of topological insulators triggered the search for new types of topological materials based on other symmetries, as represented by topological crystalline insulators where gapless SSs are protected by the space-group symmetry (specifically mirror symmetry) of crystal. Topological semimetals are recently becoming a leading material platform for realizing such novel topological states [1]. In contrast to conventional semimetals with a finite band-overlap between valence band (VB) and conduction band (CB), topological semimetals are categorized by the band-contacting nature between VB and CB in the Brillouin zone (BZ); point-contact (Dirac/Weyl semimetals) or line-contact (line-node semimetals; LNSMs). The existence of three-dimensional (3D) Dirac semimetals was first confirmed by angle-resolved photoemission spectroscopy (ARPES) where the VB and CB disperse linearly in all k axes and contact each other at the point (Dirac point) protected by rotational symmetry of the crystal. Recent ARPES studies on noncentrosymmetric transition-metal monopnictides have clarified pairs of bulk Dirac-cone bands and Fermi-arc surface states, supporting their Weyl-semimetallic nature [2]. While the existence of Weyl semimetals with point nodes has been confirmed experimentally, the experimental studies of LNSMs with line node are relatively scarce despite many theoretical predictions.

2 Experiment

High-quality single crystals of HfSiS were synthesized with a chemical vapor transport method. ARPES measurements were performed with an Omicron-Scienta SES2002 electron analyzer with energy-tunable synchrotron light at BL28A in Photon Factory. We used circularly polarized light of 36–200 eV. The energy and angular resolutions were set at 10–30 meV and 0.2°, respectively. Samples were cleaved *in situ* along the (001) crystal plane in an ultrahigh vacuum of 1×10^{-10} Torr, and kept at 30 K during the measurements.

3 Results and Discussion

We plot in Fig. 1(a) the ARPES intensity as a function of two-dimensional (2D) wave vector at the Fermi level (E_F) measured at $h\nu$ = 48 eV. One finds a "banana"-shaped Fermi surface (FS) elongated along the $\bar{X}\bar{X}$ direction, together with small pockets at $\bar{X}$. The banana-like feature gradually expands upon increasing E_B, and evolves into two diamonds at $E_B \geq 0.5$ eV, whereas the small pockets at $\bar{X}$ gradually shrink and finally disappear (not shown). The outer and inner diamonds arise from the holelike Si 3*p* and the electronlike Hf 5*d* bands, respectively.

Inside the banana-like FS, we found the additional band (X1) which is attributed to bulk band states. By switching the polarization of circularly polarized light, we also observed the X2 band (not shown) which shows the dispersion symmetric to the X1 band with respect to the $\bar{\Gamma}\bar{M}$ line. This suggests that the actual band has an X-shape tilted in *E-k* space, resulting from a merger of X1 and X2 shown in Fig. 1(b). These results led us to conclude that the X-shaped dispersion extends along a line on the $\bar{\Gamma}\bar{M}$ [black line], which can be viewed as an *arc* of Dirac node extending one-dimensionally in k space. This Dirac-node arc is apparently different from the Dirac cone of TIs and graphene where the upper and lower cones intersect at a *point* in k space. The X1 and X2 bands is insensitive to photon energy supports their surface-state (SS) origin. Obviously, these unexpected SSs pose a significant challenge in our understanding of topological LNSMs. The unexpected SSs containing a novel Dirac-node arc could be a consequence of some topology which is yet to be discovered in LNSMs. Whatever its origin, the Dirac-node arc found hear has a peculiar characteristic, that a charge neutrality point is always present in the surface state as long as the arc crosses E_F.

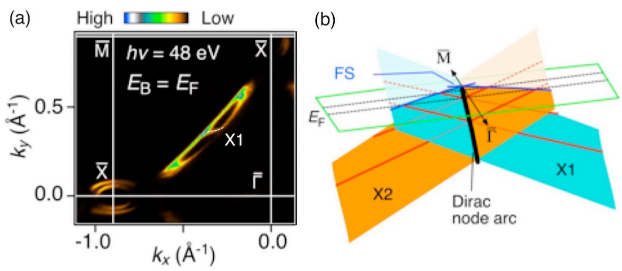

Fig. 1: (a) Fermi surface plot of HfSiS. (b) Schematic band dispersion in 3D *E-k* space for X1 and X2 band.

References

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