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A Dirac nodal line in AlB_2 observed by soft-x-ray ARPES

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1 Introduction

Topological semimetals (TSMs) host a novel quantum state of matter distinct from well-known topological insulators with a finite bulk band gap and metallic Dirac-cone surface states. Based on the way of band touching in momentum space, TSMs are categorized into two groups; point-node type (Dirac or Weyl SM) and line-node type. Topological nodal line semimetals (TNLSMs) are predicted to show unique physical properties like a flat Landau level, long-range Coulomb interaction, and unusual charge polarization and orbital magnetism. However, many of known materials realizing TNLSMs include heavy elements with large spin-orbit coupling so that band crossing points are gapped in momentum space, which would hinder the genuine physical properties relevant to nodal line.

In this regard, AlB_2 is one of most suitable materials for TNLSM because the energy bands near the Fermi level (E_F) are composed of only *s* and *p* orbitals of light elements (Al and B). AlB_2 is isostructural to well-known high-temperature superconductor MgB_2, consisting of alternatively stacking honeycomb B layers and triangular Al lattices. A first-principles band calculation suggests that AlB_2 has a linear band crossing (Dirac cone) which arises from the B sub-lattice at the K point in the bulk BZ [1], as in the case of graphene. A similar prediction is also made for iso-structural MgB_2. It is urgently required to experimentally establish the DNL in AlB_2-type materials and clarify its possible link to the exotic physical properties.

2 Experiment

High-quality single crystals of AlB_2 were grown by the Al-flux method. Angle-resolved photoemission spectroscopy (ARPES) measurements were performed with a SES2002 electron analyzer at BL2. We used linearly polarized light of 260-550 eV. The energy and angular resolutions were set to be 150 meV and 0.2°, respectively. Crystals were cleaved in situ in an ultrahigh vacuum better than 1×10^{-10} Torr along the (0001) crystal plane. Sample temperature was kept at T = 40 K during ARPES measurements.

3 Results and Discussion

By utilizing bulk-sensitive soft-x-ray photons from synchrotron radiation, we experimentally established the bulk valence band structure in the 3D bulk BZ of AlB_2, and found a highly anisotropic Dirac-cone energy band in the k_x–k_y plane which disperses along the k_z direction [2].

To elucidate the Dirac-cone band dispersion along the k_z direction, we show in Figure 1(a) the ARPES intensity

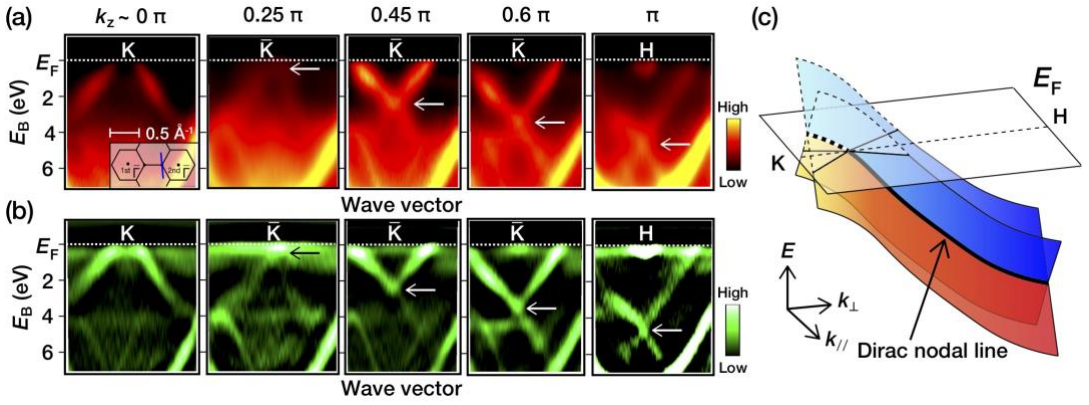

Fig. 1: (a) and (b) ARPES intensity and corresponding second-derivative intensity plots of AlB_2, respectively, measured along a cut crossing the $\bar{K}$ point for selected k_z's. Arrows indicate location of the Dirac points. (c) Schematic of the Dirac-cone dispersion and DNL around the KH line [2].

across the $\bar{K}$ point measured at various k_z's, together with the corresponding second-derivative intensity plots [Fig. 1(b)]. In Figs. 1(a) and (b), we observe a linearly dispersive band for all the k_z slices. The Dirac point located at ~ 0.5 eV above E_F at $k_z \sim 0$ gradually moves downward on increasing k_z, and finally reaches 5 eV below E_F at $k_z \sim \pi$. Intriguingly, the band always keeps the degeneracy at the $\bar{K}$ point irrespective of k_z with no indication of energy-gap opening. This firmly establishes the presence of a DNL along the whole KH line in AlB_2. The DNL has a finite slope in the E-k_z space due to the k_z dispersion of π band, as illustrated in Fig. 1(c). It is noted that we surveyed the electronic states over the entire BZ, and found no evidence for the existence of other DNLs in AlB_2. This is reasonable since the Dirac cone exists only around the $\bar{K}$ point.

It is inferred that the observed DNL in AlB_2 has the same origin as that recently predicted for MgB_2 [1], because both materials have essentially the same crystal structure and consequently the same band structure except for the position of the chemical potential (Fermi level) due to the difference in the number of valence electrons (Al has one additional electron compared to Mg). It is therefore suggested that MgB_2 also has a DNL and may behave as topological superconductor with nodal fermions contributing to the superconducting pairing. It is noted here that AlB_2 is a suitable system to investigate the anomalous transport properties originating from non-zero Berry phase, because it is theoretically proposed that the Landau orbit enclosing the KH line gives rise to the non-zero Berry phase [1]. This condition is exactly satisfied in AlB_2 [see Fig. 1(a)]. Moreover, by tuning the Al/Mg ratio in $(Al,Mg)B_2$ alloy, we are able to systematically control the electronic phase between the superconducting phase and the non-trivial Berry phase without breaking the DNL. The $(Al,Mg)B_2$ system would provide a precious opportunity to investigate the relationship between topological superconductivity and Berry phase.

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References

[1] K.-H. Jin *et al*., *npj Comput. Mater*. **5**, 57 (2019); arXiv 1710.06996 (2017).
[2] D. Takane *et al*., *Phys. Rev. B* **98**, 041105(R) (2018).

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