Surface Fermi-arc states in Weyl semimetal NbP studied by high-resolution ARPES

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1 Introduction
The Weyl semimetals (WSMs) provide a platform to realize long-sought massless Weyl fermions which can host a variety of exotic quantum phenomena like chiral anomalies and anomalous Hall conductivity [1]. The most intriguing nature of WSMs is the emergence of unconventional surface state called Fermi arc, which is distinct from the well-known Fermi surface of ordinary metals. The Fermi arc surface state must start and end at the projections of a pair of bulk Weyl cones of opposite chiralities onto the surface BZ. Recently, density functional theory predicted that transition-metal monopnictide family TaAs, TaP, NbAs, and NbP are WSMs with twelve pairs of Weyl nodes in bulk BZ [2]. These compounds crystalize in noncentrosymmetric structure, distinct from the WSM candidates which break time-reversal symmetry. To establish the WSM nature of monopnictides and to build a basis for the proposed exotic phenomena, it is of particular importance to experimentally establish the fermiology of surface state.

2 Experiment
High-quality single crystals of NbP were grown by the chemical vapor transport method. Angle-resolved photoemission spectroscopy (ARPES) measurements were performed with a VG-Scienta SES2002 electron analyzer with a tunable synchrotron light at the beamline BL28A at Photon Factory (KEK). We used circularly polarized lights of 50-200 eV. The energy and angular resolutions were set at 10-30 meV and 0.2°, respectively.

3 Results and Discussion
As shown in Fig.1, NbP crystal has two different terminations (Nb and P) because of noncentrosymmetric and polar nature of crystal. We found that such two terminations do not coexist on a single cleaved surface as long as the crystal is composed of a single domain. We accumulated the ARPES data for many cleaves, and confirmed that the obtained data are always classified into two categories attributed either to the Nb-terminated (001) or the P-terminated (001) surface.

Figure 1 summarizes the ARPES results of NbP [3]. At the P-terminated surface, we observed a tadpole-shaped FS around X point (red lines), whereas such a signature is absent at the Nb-terminated counterpart (blue lines), demonstrating nonequivalent electronic states between opposite surfaces. Since the projection of Weyl nodes must appear at the intersection of FSs for opposite surfaces, we experimentally pin down the \( \mathbf{k} \) location of Weyl nodes as shown by purple and green circles. We have estimated the \( k \) distance between adjacent Weyl nodes for W2 to be 0.06 Å\(^{-1}\) in NbP, which is much smaller than that of TaAs (≈0.15 Å\(^{-1}\)) [4]. Since the distance between adjacent Weyl nodes is a good measure of the spin-orbit-coupling strength, our ARPES data suggest that the spin-orbit coupling of NbP is essentially weak. The observed nonequivalent nature of the Fermi arcs between Nb- and P-terminated surfaces suggests a possibility to control the shape of Fermi arcs by tuning surface conditions, laying foundation for the Fermi-arc engineering of WSMs. It is also remarked that the nonequivalence of the surface states should be seriously taken into account in monopnictides, as long as the surface transport and spectroscopic properties, such as quantum oscillations in magnetotransport and possible gating devices utilizing ultrathin films, are concerned.

Fig. 1: Left: crystal structure of NbP. Right: schematics of experimental FS around the X point for the Nb- and P-terminated surfaces. Bulk Weyl nodes (W1 and W2) are illustrated by circles. Arrows indicate the chirality of Weyl nodes.

References
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