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Observation of Topological Surface States and Non-symmorphic Band Degeneracy in Superconducting PdSeTe Single-crystal

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Topological semimetals with topologically non-trivial band structures have been the focus of recent theoretical and experimental studies [1-3]. Dirac semimetals (DSMs), Weyl semimetals (WSMs), and topological nodal-line semimetals are the three main sub-categories of topological semimetals, which can be characterized according to the form and degeneracy of the band crossings near the Fermi level [4]. The layered transition metal chalcogenides among the DSMs and WSMs are particularly significant for their various intriguing physical properties, such as superconductivity and charge density wave (CDW) with application potentials [5].

In this study, we have successfully synthesized high-quality single crystals of PdSeTe which is a candidate of DSM by a two-step melting method and investigated the electronic band structure as well as the superconducting properties. We performed angle-resolved photoemission spectroscopy (ARPES) of PdSeTe on the beamline HiSOR BL-1. We have done the density functional theory (DFT) calculations and found that PdSeTe hosts four-fold degenerate Dirac crossings at the A point, originating from the non-symmorphic symmetry. These band crossings form a Dirac line node along the $\Gamma - A$ direction, which is located near the Fermi level and shows almost no energy dispersion. Therefore, Dirac fermions in PdSeTe can be studied using transport measurements. To verify the surface contribution in the ARPES results, we have done $h\nu$-dependent measurements and directly confirmed the presence of surface states in PdSeTe. The observed surface-derived states match well with the DFT calculation for the slab model.

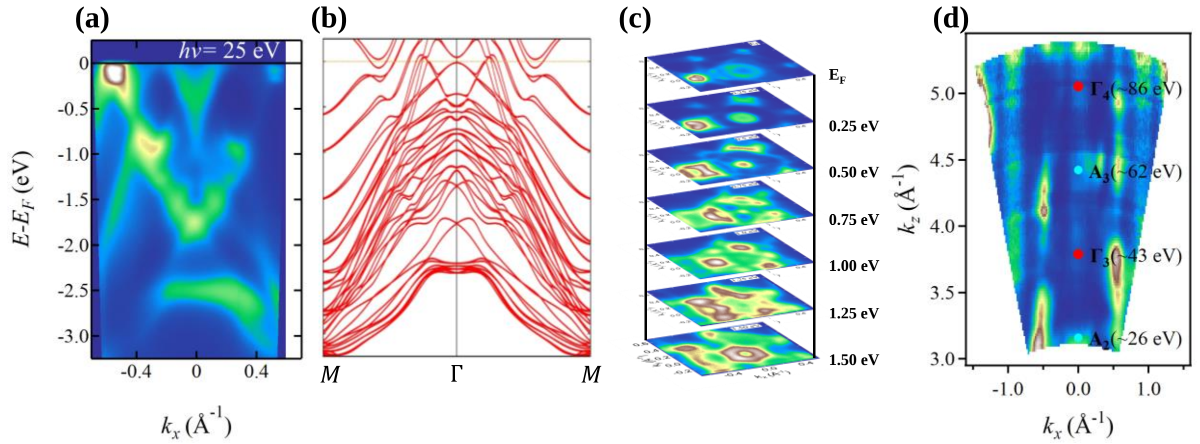

Fig. 1: (a) and (b) represent the measured ARPES spectrum along $\bar{M} - \bar{\Gamma} - \bar{M}$ direction with 25eV photon energy at 20K and simulated bands for slab (5 atomic layers) respectively. (c) The Fermi surface and constant-energy contours of the ARPES spectra at different binding energies. (d) The shows the experimental k_z-dispersion along $\Gamma - A$ deduced from the $h\nu$-dependent data measured along the $\bar{M} - \bar{\Gamma} - \bar{M}$ direction.

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