22AG001, 22AU002 BL-1 (HiSOR)

Exploration of Novel Topological Semimetal and Evolution of the Electronic Structure Using High-Resolution ARPES

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Keywords: Weyl semimetal, superconductivity, ARPES study, DFT calculation

Topological semimetals (TSMs) with the non-trivial topology of the band structure have been the focus of recent theoretical and experimental studies [1]. Depending on the shape and degeneracy of the band crossings around the Fermi level, TSMs can be mainly classified into the Dirac semimetals (DSMs), Weyl semimetals (WSMs) and topological nodal-line semimetals (NLSMs). In particular, WSMs represent a novel quantum state of matter, characterized by the presence of massless chiral particles acting as magnetic monopoles in the bulk (Weyl Fermions), and the discontinuous Fermi arcs in the topological surface states [2]. WSMs also offer interesting prospects for applications because they have the ultrahigh mobility of charge carriers and very high negative magnetoresistance due to the Adler-Bell-Jackiw anomaly [3]. The WSM concept was theoretically proposed by Wan *et al.* in 2011 [4], and one can realize it by breaking either time-reversal symmetry or spatial inversion symmetry. The WSMs are classified as either Type-I or Type-II. Type-I WSMs such as TaAs respect the Lorentz symmetry, whereas Type-II WSMs such as WTe_2 and $MoTe_2$ do not. In contrast to Type-I WSMs, the main magneto-transport feature of Type-II WSMs is the anisotropic chiral anomaly [5].

Here we examine the type-II Weyl semimetal PdSeTe and $PdTe_2$ with the CdI_2-type crystal structure [6] which is the trigonal family of the lattice with the space group $P\bar{3}m1$ (164) [7,8]. PdSeTe is non-symmorphic because it has screw axis and glid plane. PdSeTe and $PdTe_2$ are superconductors with a transition temperature of T_C ~2.74 K [8] and T_C ~1.78 K [9], respectively. We have grown high-quality PdSeTe single crystals by a two-step modified Bridgman method. We characterized the samples by the powder and single crystal X-ray diffraction (XRD) of the as-grown PdSeTe sample using a Rigaku SmartLab X-ray diffractometer with CuK_α radiation (λ =1.5406 Å). To determine the lattice parameters, we have performed Rietveld refinement using FullProf software of the XRD patterns for PdSeTe powder sample as shown in Fig. 1(a). The XRD results showed the reduction in unit cell volume from $PdTe_2$ by 10% due to Se substitution. Previous study indicated T_C of $PdTe_2$ was increased by applying pressure [10]. Since PdSeTe has slightly less unit cell volume to $PdTe_2$, we assume that the T_C was enhanced by the chemical pressure. Another possibility for the T_C enhancement could be lattice disorder or structural defects caused by Se doping. Recent study indicated that the T_C of the TaS_2 superconductor was enhanced from 2.89 K to 3.61 K due to the disorder arising from the structural defects [11].

Fig. 1(c) shows PdSeTe ARPES spectrum taken at BL-1, HiSOR. We obtained (001) clean surface by cleaving in ultrahigh vacuum. Near the Fermi level, one can see electron-like band at the $\bar{\Gamma}$ point and hole-like band at ~0.5 $Å^{-1}$. Based on the photon energy dependent measurements, we found that the band dispersion was highly two dimensional. Therefore, we have done the density functional theory (DFT) calculation for a five PdSeTe layers with the spin-orbit coupling as shown in Fig. 1(a). One can see some correspondence between the ARPES and DFT results though there are many bands in the calculation. In order to simulate ARPES spectral features we should take into account the mean-free-path of photoelectron and lifetime effect.

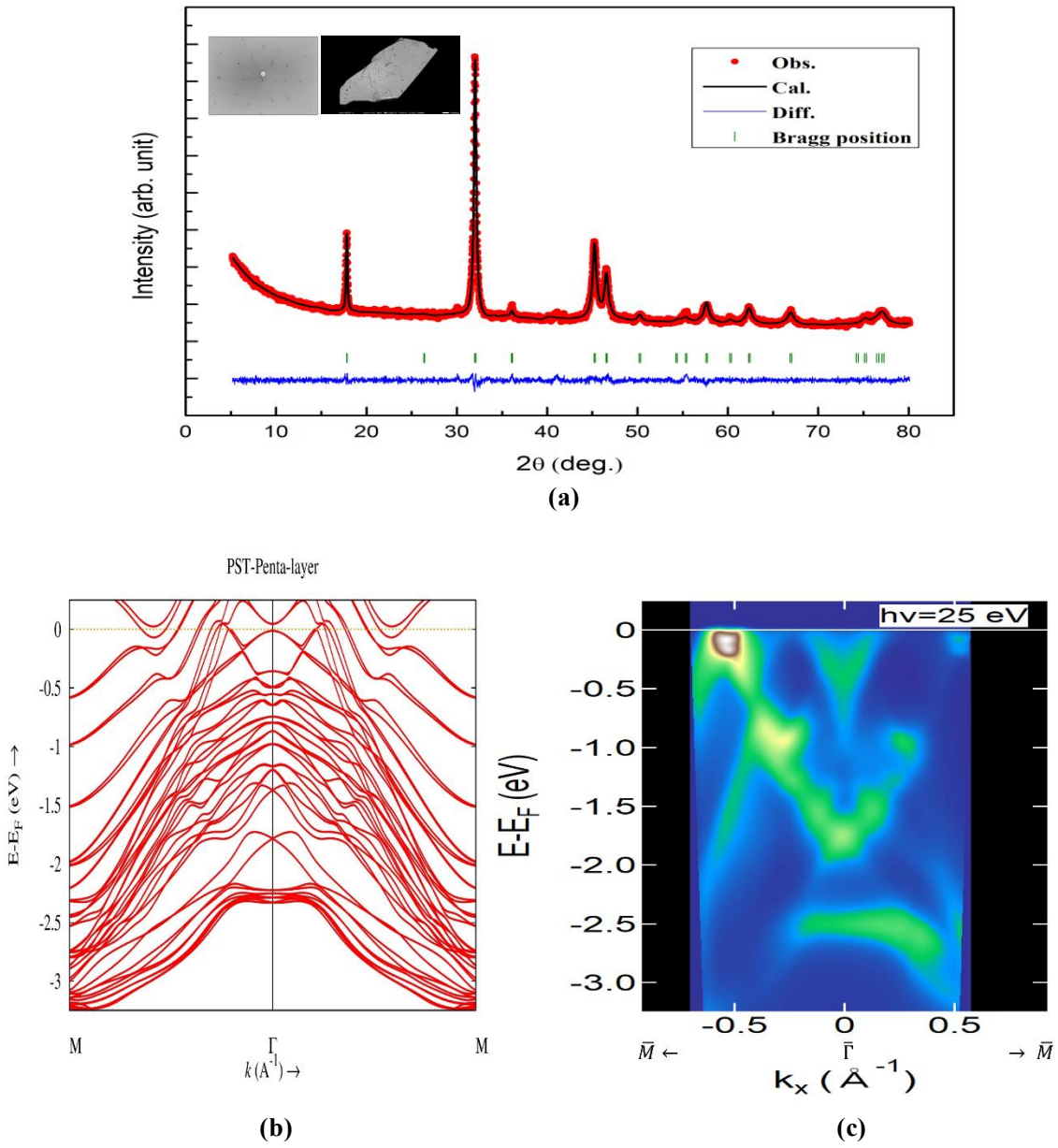

FIGURE 1. *(a) Rietveld refinement profiles of X-ray diffraction data of the PdSeTe powder sample. Insets show the Laue's diffraction pattern for (001) surface and image of the as-grown PdSeTe crystal. (b), (c) represents the simulated bands for slab (5 atomic layers) and measured ARPES spectrum along M-Γ-M direction.*

REFERENCES

[1] M. Z. Hasan and C. L. Kane, *Rev. Mod. Phys.* **82**, 3045–3067 (2010).
[2] S. Jia, S-Y. Xu and M. Z. Hasan, *Nature Materials* **15**,1140–1144 (2016).
[3] H. B. Nielsen and M. Ninomiya, *Phys. Lett. B* **130**, 389–396 (1983).
[4] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, *Phys. Rev. B* **83**, 205101 (2011).
[5] T. Nag and S. Nandy, *J. Phys.: Condens. Matter* **33** 075504 (2021).
[6] L. Thomassen, *Z. Phys. Chem. B* **2**, 349 (1929).
[7] E. McCarron, R. Korenstein, A. Wold, *Materials Research Bulletin* **11**, 1457-1462 (1976).
[8] W. Liu, S. Li, H. Wu, N. Dhale, P. Koirala, and B. Lv, *Phys. Rev. Materials* **5**, 014802 (2021).
[9] J. Guggenheim, F. Hulliger, and J. Müller, *Helvetica Physica Acta* **34**, 408 (1961).
[10] H. Leng, A. Ohmura, L. N. Anh, F. Ishikawa, T. Naka, Y. K. Huang and A. de Visser, *J. Phys. Condens. Matter* **32**, 025603 (2020).
[11] J. Peng, Z. Yu, J. Wu, Y. Zhou, Y. Guo, Z. Li, J. Zhao, C. Wu, and Y. Xie, *ACS Nano* **12**, 9461 (2018).