Anisotropic transport and de Haas–van Alphen oscillations in quasi-one-dimensional TaPtTe$_5$

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Because of the unique physical properties and potential applications, the exploration of quantum materials with diverse symmetry-protected topological states has attracted considerable interest in the condensed-matter community in recent years. Most of the topologically nontrivial materials identified thus far have two-dimensional or three-dimensional structural characteristics, while the quasi-one-dimensional (quasi-1D) analogs are rare. Here we report on anisotropic magnetoresistance, Hall effect, and quantum de Haas–van Alphen (dHvA) oscillations in TaPtTe$_5$ single crystals, which possess a layered crystal structure with quasi-1D PtTe$_2$ chains. TaPtTe$_5$ manifests an anisotropic magnetoresistance and a nonlinear Hall effect at low temperatures. The analysis of the dHvA oscillations reveals two major oscillation frequencies (63.5 T and 95.2 T). The corresponding light effective masses and the nonzero Berry phases suggest the nontrivial band topology in TaPtTe$_5$, which is further corroborated by the first-principles calculations. Our results suggest that TaPtTe$_5$, in analogy with its sister compounds TaPdTe$_5$ and TaNiTe$_5$, is another quasi-1D material hosting topological Dirac fermions.

I. INTRODUCTION

The layered ternary transition metal tellurides $MM’$Te$_4$ ($M = \text{Nb, Ta} ; M’ = \text{Ir, Rh}$), as a new class of topological materials, were theoretically proposed to host Weyl fermions $^{[1, 2]}$. Soon after, TaIrTe$_4$ and NbIrTe$_4$ were experimentally identified as type-II Weyl semimetals, with tilted Weyl cones located at the boundaries between electron and hole pockets by breaking the Lorentz invariance $^{[3, 7]}$. The layered structure as well as weaker van der Waals interlayer interaction than that in graphite $^{[2]}$, facilitates mechanical exfoliation and thus device fabrication, making them an ideal platform for exploring device applications and exotic properties in low-dimensional topological semimetals.

The quasi-one-dimensional (quasi-1D) topologically nontrivial materials are thus far sparse and claimed to host highly anisotropic surface-state Dirac/Weyl fermions $^{[3, 6, 8]}$. A complex electronic structure can be tuned, for example, in quasi-1D topological insulator $\beta$-Bi$_2$I$_4$ by external pressure, to study the competing or even cooperative interplay of topological physics, electronic instability, and superconductivity $^{[3]}$. Recently, we reported the synthesis and characterizations of a new layered ternary Pd-based telluride TaPdTe$_5$ with quasi-1D PdTe$_2$ chains $^{[10]}$, the advent of which enriches further the family of layered ternary transition metal tellurides. Interestingly, by analyzing the de Haas–van Alphen (dHvA) oscillations, we observed the typical signatures of Dirac fermions, which indicates TaPdTe$_5$ is a new topologically nontrivial material. The first-principles calculations further verified topologically nontrivial states therein. The structural similarity with the other two ternary Pd-based telluride superconductors Ta$_4$Pd$_3$Te$_{16}$ and Ta$_3$Pd$_4$Te$_{14}$ $^{[11, 12]}$, leads us to conjecture that more exotic properties, e.g., topological superconductivity, may exist in this low-dimensional Pd-based telluride system. The sister compound TaNiTe$_5$, crystalizing in the same space group $Cmcm$, was theoretically predicted to be topologically nontrivial $^{[13]}$. Later,
Xu et al. and Chen et al. independently reported the experimental evidence of the nontrivial band topology in TaNiTe$_5$ [14, 15]. The layered nature and weak interlayer binding energies of this new family of ternary layered tellurides with quasi-1D chains make them a promising platform for exploring the nature of both topological and superconducting phases.

Another layered ternary transition metal telluride TaPtTe$_5$ isostructural with TaPdTe$_5$ and TaNiTe$_5$ was synthesized in 1991 and reported to be a good metal with Pauli-paramagnetism [16]. However, the experimental results of its transport properties and electronic structure remain unreported. In this work, we report the transport properties along three crystallographic directions. The seemingly unsaturated magnetoresistance is found to be anisotropic and the non-linear Hall effect at low temperatures indicates TaPtTe$_5$ be anisotropic and the non-linear Hall effect at low temperatures indicates TaPtTe$_5$ is another example of layered topological semimetal with quasi-1D chains, like TaPdTe$_5$ and TaNiTe$_5$, and is thus suitable for the study of the interplay between dimensionality and nontrivial topology and even the topological superconductivity.

II. EXPERIMENTAL METHODS

A. Sample synthesis

Single crystals of TaPtTe$_5$ were grown in Te solution as reported previously [16]. Powders of the elements Ta (99.97%), Pt (99.98%), and Te (99.99%) with a molar ratio of Ta : Pt : Te = 1 : 1 : 10, were thoroughly mixed together in a glove box filled with highly pure argon gas, and then sealed into an evacuated quartz ampule. The quartz ampule was firstly heated up to 773 K and held for 24 h, and then heated to 1073 K and held for another 24 h. Before being cooled down to room temperature for 24 h, the ampule was quickly heated to 1273 K and held for 4 days. The obtained air-stable crystals show a shiny gray-black flattened needle-like shape with the typical dimensions of $2.5 \times 0.3 \times 0.1$ mm$^3$ [see the left inset of Fig. 1(b)]. The heating process adopted in growing its isostructural TaPdTe$_5$ crystals [10], was unsuccessful in growing TaPtTe$_5$ crystals.

B. Composition determination

The chemical composition was measured by energy-dispersive x-ray spectroscopy (EDS) with an A M E T E K©EDAX (Model Octane Plus) spectrometer, equipped in a field-emission scanning electron microscope.
(SEM) (Hitachi S-4800). The EDS analysis was performed on the fresh surface cleaved from the selected crystals, which gives the average composition being \(\text{Ta}_{1.03}\text{Pt}_{1.01}\text{Te}_{4.96}\), very close to the stoichiometric one \(\text{TaPtTe}_5\). Taking into consideration the measurement precision, we expect there is no significant deficiency at any atomic sites. The typical EDS spectrum for a piece of crystal is shown in Fig. 1(b). The SEM image, shown in the right inset of Fig. 1(b), reveals a morphology with stripes along the \(a\) axis, consistent with the preferential crystal growth along the chain direction.

X-ray diffraction (XRD) data acquisition was performed at room temperature with a monochromatic Cu \(K_{\alpha 1}\) radiation using a PANalytical x-ray diffractometer (model EMPYREAN) radiation by a conventional \(\theta-2\theta\) scan for a crystal lying on a sample holder. The XRD pattern at 298 K is shown in Fig. 1(a), from which only multiple peaks arising from the diffraction from (010) planes can be observed, consistent with the layered crystal structure of \(\text{TaPtTe}_5\). The full width at half-maximum is only 0.05°, e.g., for the (0100) peak, indicating high quality of the crystals. The interplane spacing is calculated to be 6.630 Å, close to half of the lattice parameter \(b\) \((b/2 = 6.616 \text{ Å})\) at 111 K as reported in Ref. [10]. The very close lattice parameters of \(\text{TaPtTe}_5\) to those of \(\text{TaPdTe}_5\) is reasonable because the atomic radii of Pt and Pd are similar [10]. In the right inset of Fig. 1(a), we plot the calibrated fifth reflection of XRD patterns to show how close, from a perspective, the lattice parameters of them are.

C. Physical property measurements

The resistivity and low-field magnetoresistivity measurements were carried out in a physical property measurement system (PPMS-9, Quantum Design) with dc transport option. A standard four-probe method was employed for the resistivity measurements. The Hall-effect measurement was performed by reversing the field direction and antisymmetrizing the data. Magnetic susceptibility measurements were performed on a commercial Quantum Design magnetic property measurement system (MPMS-7).

D. Band structure calculations

The electronic structure calculations with high accuracy were performed using the full-potential linearized augmented plane wave (FP-LAPW) method implemented in the WIEN2K code [17]. The generalized gradient approximation (GGA) presented by Wu and Cohen [18] was applied to the exchange-correlation potential calculation. The muffin tin radii were chosen to be 2.5 a.u. for all atoms. The plane-wave cutoff was defined by \(RK_{\text{max}} = 7.0\), where \(R\) is the smallest of all atomic sphere radii and \(K_{\text{max}}\) is the plane wave cut-off. We also constructed a tight-binding model Hamilton to analyze the topological properties of \(\text{TaPtTe}_5\). The tight-binding model matrix elements were calculated by projecting onto the Wannier orbitals [19]. We used \(\text{Ta} d, \text{Pt} d\), and \(\text{Te} p\) orbitals to construct Wannier functions. The topological invariants \(Z_2\) were calculated by the surface Green’s function methods as implemented in WannierTools [20].

III. RESULTS AND DISCUSSION

The temperature \((T)\) dependence of electrical resistivity measured at zero field along three crystallographic directions is shown in Fig. 2(a). A typical metallic behavior with an in-chain residual resistivity ratio \(\text{RRR} = \rho_0(300 \text{ K})/\rho_0(2 \text{ K}) = 15\) is observed. The resistivity almost follows a \(T\) dependence of electrical resistivity anisotropy for \(\rho_c/\rho_a\) and \(\rho_b/\rho_a\). The inset of Fig. 2(b) plots the \(T\) dependence of anisotropic ratios \(\rho_b/\rho_a\) and \(\rho_c/\rho_a\). The most conducting direction is reasonably along the chain direction and anisotropic transport behaviors are manifested by \(\rho_a : \rho_b : \rho_c = 1 : 10.6 : 1.3\) at 300 K, and \(1 : 12.6 : 1.6\) at 2 K. The much smaller anisotropic values than those of \(\text{TaPdTe}_5\) and \(\text{TaNiTe}_5\) [10] suggest the stronger interchain coupling in \(\text{TaPtTe}_5\). A broad maximum of the anisotropy is observed around 45 K for both \(\rho_b/\rho_a\) and \(\rho_c/\rho_a\), a similar behavior of which also appears in \(\text{TaPdTe}_5\), but only for \(\rho_c/\rho_a\) at a lower temperature [10].

The \(T\)-dependent transverse magnetoresistance (MR)
under different current and field configurations is shown in Figs. 3(a)–3(c). The MR of \( \rho_a \) and \( \rho_b \) basically shows the similar \( T \)-dependent behavior, while being obviously different from that of \( \rho_c \). The MR of \( \rho_c \) above a threshold field \( 5 \) T begins to increase below a ‘turn on’ temperature \( T^* \), defined as the temperature at which a resistivity minimum appears, and saturates to a plateau with further decreasing temperature. The ‘turn on’ temperature linearly increases with increasing the applied magnetic field at the rate of \( 4.2 \) K/T, as shown in the inset of Fig. 3(c). The similar magnetic-field-driven metal-insulator transition has been observed in several topological semimetals \cite{3, 11, 21, 22}, possibly due to the Landau level quantization of relativistic quasiparticles by the magnetic field \( 21, 22 \). The other possible explanation is a metal-insulator transition as in trivial semimetals \cite{23, 24}, when close to perfect charge carriers compensation, as discussed for WTe\(_2\) \cite{23}. The corresponding field-dependent MR ratio, \( \rho(H)/\rho(0) \), is displayed in Figs. 3(d)–3(f). The quantitative behavior of \( \Delta\rho_c/\rho_c \) is similar, both of which at \( 2 \) K can be fitted to a single power law \( \propto H^\alpha \) with \( \alpha = 1.58 \) and 1.53, while the field evolution of \( \Delta\rho_a/\rho_a \) at \( 2 \) K is very different, which, in combination with the Hall resistivity as discussed below, can otherwise be described by a two-band model \cite{20}. Our attempt to attribute the data to the mixture of Dirac-like linear MR and conventional quadratic MR is unsuccessful in contrast with that of the isostructural TaPdTe\(_5\) \cite{10}. The pronounced positive \( \Delta\rho_c/\rho_c \) is as well manifested in Fig. 3(f), and reaches \( 164\% \) at \( 9 \) T, nearly two times larger than \( \Delta\rho_b/\rho_b \) (92.4\%) and over five times larger than \( \Delta\rho_a/\rho_a \) (30.5\%). The significant anisotropic transport reflects the anisotropic Fermi surfaces, as evidenced by our first-principles calculations shown below, and the associated anisotropic transport lifetime. The Kohler’s plots for the three configurations are shown in Figs. 3(g)–(i). For \( \rho_b \) and \( \rho_c \), the Kohler’s rule is basically obeyed over a large temperature range, while for \( \rho_a \), it is moderately violated, presumably due to the influence from Dirac electrons or anisotropic carrier scattering time.

The results of Hall resistivity (\( \rho_{xy} \)) measurements, performed with the electric current flowing along the \( a \) axis and magnetic field applied along the \( b \) axis at selected temperatures below \( 200 \) K, are shown in Fig. 4(a). Nonlinear field-dependent \( \rho_{xy} \) can be clearly observed, especially at temperatures below \( 20 \) K, reflecting the multiband character of the electrical transport in TaPdTe\(_5\). At high temperatures (\( T \geq 60 \) K), \( \rho_{xy} \) is still positive and develops linearly with the field, indicating the single hole-type carriers dominate the transport. The positive value of \( \rho_{xy} \) in the temperatures investigated indicates the dominance of hole-type charge carriers, consistent with our first-principles calculations. To
plotted in Fig. 4(c), e.g., fitting parameters derived in the above approach are
where $n_b/n_e = 4.4$. Therefore, our result clearly excludes the possibility of electron-hole compensation effect in TaPtTe$_3$, similar to that in the sister compound TaPdTe$_3$ [10]. The $T$-dependent Hall coefficient $R_H$ is plotted in the inset of Fig. 4(a), obtained by the linear fitting with the corresponding $\rho_{xy}$ below 1 T. The obvious $T$-dependent $R_H(T)$ also signals multiple bands with coexisting hole and electron pockets.

In Fig. 4(a), we present the isothermal magnetization measured up to 7 T under $H \parallel b$ for TaPtTe$_3$. The dHvA quantum oscillations can be clearly observed when the magnetic field exceeding 3.5 T at 1.8 K, and can sustain up to 14 K. We also measured the isothermal magnetization under $H \parallel a$ and $H \parallel c$ (data not shown here), however, no clear quantum oscillations could be seen up to 7 T, suggesting the Fermi pocket associated with the dHvA oscillations under $H \parallel b$ is from 2D-like Fermi surface. The oscillatory magnetization, obtained after subtracting the background, are presented in Fig. 5(b). Moderate oscillations with the amplitudes of $1.6 \times 10^{-3}$ emu/g at 1.8 K, much weaker than that of the isostructural compound TaPdTe$_3$ under $H \parallel a$ [10], are clearly seen. From the fast Fourier transform (FFT) analyses of the oscillatory magnetization, we derived two major oscillation frequencies $F_\alpha = 63.5$ T and $F_\beta = 95.2$ T in Fig. 5(c). By assuming the circular cross section of the Fermi surface along [010], the cross-sectional Fermi area (AF) can be calculated from Onsager relation $S = 4\pi \rho_{xy} F / H$, where $F$ is the frequency of oscillation. The two corresponding $S$ are $S_\alpha = 6.05 \times 10^{-3}$ Å$^{-2}$ and $S_\beta = 9.07 \times 10^{-3}$ Å$^{-2}$. The obtained $S$ is used further to obtain the Fermi vector $k_0 = \sqrt{S_\alpha/\pi} = 4.39 \times 10^{-2}$ Å$^{-1}$ and $k_\beta = \sqrt{S_\beta/\pi} = 5.37 \times 10^{-2}$ Å$^{-1}$. In general, the oscillatory dHvA magnetization can be described using the Lifshitz-Kosevich (LK) formula [27], which takes the Berry phase into account for a Dirac system [28]:

$$\Delta M \propto -R_T \cdot R_D \cdot R_S \cdot \sin \left[ 2\pi \frac{F}{\mu_0 H} - \gamma - \delta \right],$$

where $R_T = \frac{2\pi^2 k_B T \mu_{\text{loc}}^2}{\sinh(2\pi^2 k_B T \mu_{\text{loc}} H / \hbar \mu_0)},$ $R_D = \exp(2\pi^2 k_B T D \mu_{\text{loc}} H / \hbar \mu_0),$ and $R_S = \cos(\pi \gamma / 2 \mu_0),$ are the thermal damping factor, Dingle damping term, and a spin-related damping term, respectively. $T_D$ is the Dingle temperature. The oscillation of $\Delta M$ is described by the sine term with the phase factor $-\gamma - \delta$, in which $\gamma = \frac{1}{2} - \frac{\phi_\text{B}}{2 \pi}$ and $\phi_\text{B}$ is the Berry phase. The additional phase shift $\delta$ is determined by the dimensionality of the FS, and is equal to 0 and ±1/8 (− for the electronlike and + for the holelike), respectively, for the 2D and 3D

FIG. 5. (Color online) The dHvA oscillations in TaPtTe$_3$. (a) Isothermal magnetization under $H \parallel b$ at different temperatures from 1.8 K to 14 K. (b) The magnetization oscillations at different temperatures after subtracting the background. (c) The corresponding FFT spectrum. (d) The FFT amplitude as a function of temperature and the fit to $R_T$ to determine the effective mass. (e) The Lifshitz-Kosevich fit (green line) of the oscillation pattern and the extracted single-frequency oscillatory part at 1.8 K. The single-frequency parts are shifted by $2.5 \times 10^{-3}$ emu/g respectively for clarity. (f) The Landau’s fan diagram for the identified frequency. The n-axis intercept is illustrated in the inset.

quantitatively analyze the experimental data, we apply a simplified two-band Drude model including one electron-type band and one hole-type band [20]. First, the data of $\rho_{xy}(\mu_0 H)$ measured below 20 K are converted to the Hall conductivity $\sigma_{xy} = \rho_{xy}/(\rho_{xx}^2 + \rho_{xy}^2)$, as displayed in Fig. 3(b) (the data at 10 K not shown here for clarity). Then, $\sigma_{xy}(\mu_0 H)$ was fitted by the formula

$$\sigma_{xy} = e\mu_0 H \left[ \frac{n_h \mu^2}{1 + (\mu_h \mu_0 H)^2} + \frac{n_e \mu^2}{1 + (\mu_e \mu_0 H)^2} \right],$$

where $e$ is the absolute value of elementary charge, $n_e(h)$ and $\mu_e(h)$ are the carrier densities and mobilities of the electrons (holes), respectively. The fit is well performed, as evidenced by the red fitting lines in Fig. 3(b). The fitting parameters derived in the above approach are plotted in Fig. 3(c), e.g., $n_h = 3.41 \times 10^{20}$ cm$^{-3}$ and $n_e = 7.83 \times 10^{19}$ cm$^{-3}$, $\mu_h = 1113$ cm$^2$ V$^{-1}$ s$^{-1}$ and $\mu_e = 3007$ cm$^2$ V$^{-1}$ s$^{-1}$ at 2 K. The hole-like carrier density in the $T$ interval we studied is nearly five times larger than the electron-like carrier density. However, the mobility of electrons is almost three times larger than that of holes. With regard to the level of carrier compensation, the two-band model yields considerable charge imbalance given by the ratio $n_h/n_e = 4.4$. Therefore, our result clearly excludes the possibility of electron-hole compensation effect in TaPtTe$_3$, similar to that in the sister compound TaPdTe$_3$. The $T$-dependent Hall coefficient $R_H$ is plotted in the inset of Fig. 4(a), obtained by the linear fitting with the corresponding $\rho_{xy}$ below 1 T. The obvious $T$-dependent $R_H(T)$ also signals multiple bands with coexisting hole and electron pockets.
cases. The fit of the $T$ dependence of the FFT amplitude to the thermal damping factor $R_T$ yields effective masses corresponding to two fundamental frequencies $m_\alpha^* = 0.108 m_e$ and $m_\beta^* = 0.119 m_e$ ($m_e$ is the free electron mass), as shown in Fig. 5(d). With the fixed parameters of two fundamental frequencies and corresponding effective masses, the oscillation pattern can be well fitted using the LK formula. The extracted single-frequency oscillatory parts are plotted separately in Fig. 5(e), and the LK formula basically reproduces the oscillations at 1.8 K, yielding $T_D = 10.99$ K for the $F_\alpha$ band and $T_D = 24.68$ K for the $F_\beta$ band, which correspond to the quantum relaxation time $\tau_\eta = h/(2\pi k_B T_D) = 1.11 \times 10^{-13}$ s ($F_\alpha$), $0.49 \times 10^{-13}$ s ($F_\beta$) and quantum mobility $\mu_\eta = e\tau/m^* = 1800$ cm$^2$ V$^{-1}$ s$^{-1}$ ($F_\alpha$), $727$ cm$^2$ V$^{-1}$ s$^{-1}$ ($F_\beta$). The phase factors of $\gamma - \delta$ are fitted to be $1.10$ ($F_\alpha$) and $0.83$ ($F_\beta$), from which the Berry phases $\varphi_B$ are derived to be $-0.20\pi$, $-0.45\pi$, and $0.05\pi$ ($F_\alpha$) and $0.33\pi$, $0.08\pi$, and $0.58\pi$ ($F_\beta$) for $\delta = 0$, $-1/8$, and $1/8$, respectively. In general, the Berry phase is zero for a parabolic energy dispersion and $\pi$ for a linear energy dispersion. A finite Berry phase, deviating from the exact $\pi$ value, is also possible due to the deviation of the dispersion relation $E(k)$ from an ideal linear dispersion \cite{29}. The Berry phase can be also evaluated using the Landau level (LL) fan diagram \cite{30}. The minima of $\Delta M$ should be assigned to a LL index of $n - 1/4$. The established LL fan diagram is shown in Fig. 5(f). The linear extrapolations in the fan diagram yield two intercepts $n_0 = -0.076 \pm 0.005$ ($F_\alpha$) and $n_0 = 0.015 \pm 0.01$ ($F_\beta$), corresponding to a nontrivial Berry phase of $\varphi_B = 2\pi (-0.076 + \delta) (F_\alpha)$ and $\varphi_B = 2\pi (0.015 + \delta) (F_\beta)$. The slopes of the LL indices are $63.4$ T and $95.2$ T for the $F_\alpha$ band and $F_\beta$ band, in excellent agreement with the frequencies obtained from FFT analysis.

To obtain a comprehensive understanding of the topological electronic properties of TaPtTe$_5$, we calculated the bulk and surface electronic structure. The calculated band structures both without and with spin-orbit coupling (SOC) are shown in Figs. 6(a) and 6(f), with four bands crossing the Fermi level marked by different colors. The major change that can be found when SOC is introduced is that the gap between band 2 and band 3 is significantly shrank. The presence of electron and hole pockets located at the Fermi level is consistent with the nonlinear Hall resistivity observed experimentally. The band structures show different dispersions around high-symmetry points $Z$ and $T$. Similar to that of the quasi-1D compounds TaPdTe$_5$ and Tl$_2$Mo$_6$Se$_9$ \cite{10, 31, 32}, the band structures of TaPtTe$_5$ also show cubic Dirac dispersion along $Z$-$T$, but linear characteristic along $T$-$Z$ and $T$-$Y$, as shown in Fig. 6(f). The blue arrows indicate the cubic Dirac dispersion between the high symmetry points: $Z(0, 0, 0.5)$ and $T(0.5, 0.5, 0.5)$, and the standard linear Dirac dispersion along $\Gamma(0, 0, 0)$-$Z(0, 0, 0.5)$ and $T(0.5, 0.5, 0.5)$-$Y(0.5, 0.5, 0)$. As the three compounds TaNiTe$_5$, TaPdTe$_5$, and TaPtTe$_5$ are isostructural, it is meaningful to make a comparison of the band structures. One significant change we found is that the conduction band around the point $S$ gradually passes through the Fermi level upward as the intermediate transition-metal element getting heavier (data not shown here). The bulk Fermi surfaces for each

![FIG. 6. (Color online) Band structure for orthorhombic TaPtTe$_5$. (a) Without SOC and (f) with SOC. The band structures show different dispersions around high-symmetry points $Z$ and $T$. (b)–(e) Fermi surface for each band, without SOC. (g)–(j) Fermi surface for each band, with SOC. The arrows indicate the extremal orbits from the corresponding sheets. (k) Surface-state spectrum of TaPtTe$_5$ in the presence of SOC along high-symmetry $k$ line $\Gamma$-$T$-$\Gamma$. The bright red lines denote the surface states. (l) Bulk and surface projected Brillouin zone (BZ) with the high-symmetry points specified.](image)
band are visualized in Figs. 6(b)–6(e) (without SOC) and in Figs. 6(g)–6(j) (with SOC). The Fermi surface of band 1 and band 2 changes significantly with SOC, i.e., the Fermi surface of band 1 gets smaller with SOC included, and a hollow cavity appears at the center of the Fermi surface of band 2. As a whole, the Fermi surfaces exhibit weak dispersions along the \( \Gamma - Y \) direction (the crystallographic \( b \) axis in the real space), indicating a noticeable 2D character. The extremal-orbit dHvA frequencies of the calculated Fermi surfaces were also analyzed to make a comparison with our experiment. Along the \( \Gamma - Y \) direction, two extremal orbits from the Fermi surface sheet of the band 1 are corresponding to the two frequencies 76.7 T and 299.9 T, indicated by the red and green lines in Fig. 6(g). The small cross-sectional area can be well assigned to the experimentally observed frequency \( F_3 \). However, the measured frequency \( F_3 \) differs by \( \sim 200 \) T from the calculated second frequency. The calculated Fermi surface also suggests one more frequency, corresponding to the larger extremal orbits arising from the band 2, indicated by the blue line in Fig. 6(h). Much lower temperatures and higher magnetic fields might enable its observation. Certainly, refinement of the present picture of the Fermi surface sheets may be helpful to reconcile with the experimental results. The topological nontriviality can be evaluated by \( Z_2 \) topological indices (\( \nu_0; \nu_1; \nu_2; \nu_3 \)). We have calculated the \( Z_2 \) topological number, which is valid for time-reversal invariant system. The \( Z_2 \) topological number for 3D bulk system can be obtained from the calculation of the Wilson loop for the gap between the highest occupied and lowest unoccupied bands in the six time-reversal invariant momentum plane: \( k_x = 0, \pi/a; k_y = 0, \pi/b; \) and \( k_z = 0, \pi/c \). The calculated \( Z_2 \) is 1 for \( k_x = 0, \pi/a; k_y = 0, \pi/b; \) while zero for \( k_z = 0, \pi/c \). The corresponding topological index is \( (0; 110) \), which indicates that TaPtTe\(_5\) is a weak topological material. The calculated surface state spectrum along \( Y - \Gamma - Y \) is plotted in Fig. 6(k), from which a Dirac-cone-like linear surface state at the \( \Gamma \) point can be observed (indicated by the red arrow). The Dirac-cone-like surface bands emerge in the gap around the point \( \Gamma \) between the band 1 and the subjacent occupied bands, the topological index of which is calculated to be \( (1, 110) \), indicating a topologically nontrivial surface state.

IV. SUMMARY

To summarize, we have successfully synthesized the high-quality single crystals of a layered ternary telluride TaPtTe\(_5\). The layered structure is composed of alternative PtTe\(_2\) and TaTe\(_3\) chains. Anisotropic MR for the current and the magnetic field applied along different crystallographic directions reflects anisotropic Fermi surfaces, originating from the low-dimensional crystal structure. The light effective masses of charge carriers, the nontrivial Berry phases revealed by the dHvA oscillations and the first-principles calculations verify TaPtTe\(_5\) is a topologically nontrivial material. The easily exfoliated thin layers make TaPtTe\(_5\) another ideal platform for device applications and studying the nontrivial physics in low dimensions. More experiments, such as the angle dependent dHvA oscillations, angle-resolved photoemission spectroscopy, are invoked to provide further insights into its Fermiology and the topological properties. It would be also intriguing to explore the possible topological superconductivity in this class of materials by chemical substitution, voltage gating, or the high pressure, when noting that the ternary tellurides Ta\(_5\)Pd\(_3\)Te\(_{16}\) and Ta\(_5\)Pd\(_3\)Te\(_{14}\) with similar structural characteristics are superconductors, while the ternary tellurides TaIrTe\(_4\), TaPdTe\(_5\), TaNiTe\(_5\), and TaPtTe\(_5\) are topological materials.

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