Large Magnetoresistance in Topological Insulator Candidate TaSe$_3$

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Abstract

Large unsaturated magnetoresistance (XMR) with magnitude $\sim 10^3\%$ is observed in topological insulator candidate TaSe$_3$ from our high field (up to 38 T) measurements. Two oscillation modes are detected associated with the bulk pockets from our Shubnikov-de Hass (SdH) measurements, consistent with our first-principles calculations. However, our SdH measurements fails to determine the existence of topological surface states in TaSe$_3$, calling for more powerful means to detect on this compound. Moreover, our two-band model analysis exhibits that an imperfect density ratio $n_h/n_e \approx 0.9$ accounts for XMR at $T< 20$ K. At $T> 20$ K, a sudden change of density of carriers suggests a reconstruction of the Fermi surface. Thus, TaSe$_3$ may provide an opportunity to allow us to observe XMR in a topological insulator and to exploit the potential interplay between the XMR and topological surface states for the first time.
I. INTRODUCTION

Large unsaturated magnetoresistance (XMR) is an interest of transport phenomenon in solids. The magnetoresistance exhibits a dramatic augment without showing any saturating behavior even when the field reaches rather high [1-3]. From a semi-classical point of view, an interpretation says that compensation between hole and electron carriers weakens the Hall field that counteracts the Lorentz force resulting in an XMR [1]. Earlier on, XMR has been observed in a few semimetals, such as Bismuth, for hosting comparable number of hole and electron carriers [4-6]. Recently, a non-saturating XMR with magnitude \( \sim 10^{4-6\%} \) has drawn much attention again due to its common existence in topological semimetals, including Cd\(_3\)As\(_2\) [7], WTe\(_2\) [3,8-10], MoTe\(_2\) [11,12], TaAs family [13-17], lanthanum monopnictide family [18-23], etc., with exotic transport properties [24].

Nevertheless, XMR has yet been found in any topological insulators, such as Bi\(_2\)Se\(_3\) family [25], PbSn\(_{1-x}\)Se\(_x\) [26], BiTeI [27-29]. It is not hard to understand because the bulk states remains insulating at the Fermi surface for a typical topological insulator [30]. Even in an n-doped or p-doped case, the lack of XMR could be interpreted as a result of the absence of the coexistence of both hole and electron types of carriers. Interestingly, a kind of material named TaSe\(_3\) with bulk semimetallic states was recently predicted to be a strong topological insulator candidate [31]. It is a quasi-one-dimensional trichalcogenide with space group \( P2_1/m \) (No. 11) and the crystal structure are shown in Fig. 1(a). In previous works, single crystal TaSe\(_3\) yields a residual resistance ratio (RRR) around 20 [32] and TaSe\(_3\) nanowires claims a low resistivity and high breakdown current density [33-35]. In addition, TaSe\(_3\) mesowires possibly host a charge density wave (CDW) at 65 K [36]. Thus, TaSe\(_3\) may provide an opportunity to allow us to observe XMR in a topological insulator and exploit the potential interplay between the XMR and topological surface states for the first time.

Here, we systematically investigate the electronic structure of TaSe\(_3\) and its corresponding transport behavior in this material by combining the first-principles...
calculations and low-temperature and high-field transport measurements. Unsaturated XMR with magnitude $\sim 10^3 \%$ is observed from our high field (up to 38 T) measurements. Besides, two oscillation modes are detected associated with the bulk pockets from our SdH measurements, consistent with our first-principles calculations, indicating a topologically trivial electronic structure in bulk. Moreover, our two-band model analysis exhibits that an imperfect density ratio $n_h/n_e \approx 0.9$ accounts for XMR when $T<20$ K. When temperature increasing to 20 K, a sudden change of density of carriers suggests a reconstruction of the Fermi surface. However, our SdH measurements fail to determine the existence of topological surface states in TaSe$_3$ compound, calling for more powerful means to detect on this TaSe$_3$ compound in the future.

II. RESULTS AND DISCUSSIONS

A. First-principles calculations

The first-principles calculations were performed using the Vienna ab-initio simulation package (VASP) [37,38] and the generalized gradient approximation with the Perdew-Burke-Ernzerhof (PBE) [39,40] type exchange correlation potential adopted the energy cutoff fixed to 500 eV. The lattice constant $a = 9.829 \, \text{Å}$, $b = 3.495 \, \text{Å}$, $c = 10.402 \, \text{Å}$, $\alpha = \gamma = 90^\circ$, $\beta = 106.26^\circ$, and the ionic positions were relaxed until the energy tolerance was less than $10^{-6}$eV. In order to obtain the accurate band gap, we adopted a modified Becke-Johnson (mBJ) exchange potential [41] at the meta-GGA level. The $k$-point sampling grid of the Brillouin zone in the self-consistent process was a $\Gamma$-centered Monkhorst-Pack $k$-point mesh of $6 \times 15 \times 5$, and a total energy tolerance $10^{-7}$eV was adopted for self-consistent convergence. In order to compute the surface density of states, the tight-binding model of Ta–d and Se–p orbitals was constructed by the maximally localized Wannier functions (MLWF)
We performed the first-principles calculations in order to obtain the basic understandings of the topological nature of electronic structure as well as the Fermi pockets of TaSe$_3$. Fig. 1(b) displays the calculated band structure without spin-orbit coupling (SOC), noticing that a band crossing can be identified as marked by the dashed rectangle. The crossing points are gapped when inducing SOC as displayed in Fig. 1(c). By calculating the topological invariant $Z_2$ through the Wannier charge center(WCC) [47], TaSe$_3$ proves to be a strong topological insulator since the WCC of six time-reversal invariant momentum plane (Fig. 1(e)) guarantee that $Z_2 = (1; 100)$, consistent with the previous report [31]. Fig. 1(f) shows the surface states on $(0 \ 1 \ 0)$ plane of TaSe$_3$, where one Dirac cone of topological surface states lies at $\overline{B}$ point. From the view of topology classification, TaSe$_3$ is really a strong topological insulator. However, it is worth to notice that there is no real universal band gap in this system and there are bulk conduction band and valence band crossing the Fermi level simultaneously, and that the strong topological insulator state is defined based on a so-called curved Fermi level. Left panel of Fig. 1(d) shows the calculated three-dimensional Fermi surfaces, a large hole pocket enclosing the $\Gamma$ point and two electron pockets near the $B$ point are included. Their projections along $(1 \ 0 \ -1)$ direction are presented in the right panel of Fig. 1(d).

**B. Crystal growth and characterizations**

To experimentally investigate the transport properties of this topological insulator candidate TaSe$_3$, single crystals were synthesized via chemical vapor transport (CVT) method. Ta, Se powders were mixed in a ratio of 1:3 and a proper excess of Se was used as transport agent. The mixture was vacuum sealed in a quartz tube, and then heated up to high temperature with a gradient from 1000 °C to 600 °C in a two-zone furnace and kept for one week. Then the furnace was naturally cooled down and the ribbon-like crystals were obtained with typical dimensions of 5 mm × 0.1 mm × 0.05 mm, where
the longest dimension corresponds to crystallographic $b$ axis (along the Ta-Ta chains). The chemical components of the obtained TaSe$_3$ crystals were identified by the energy dispersive spectrum (EDS), as shown in Fig. 2(a). An atomic ratio Ta : Se = 1 : 2.73 could be extracted from the EDS, suggesting a slight amount of Se vacancies in our samples. The insets of Fig. 2(a) show the EDS mapping of Ta and Se, indicating the uniform distribution of the two elements in the obtained TaSe$_3$ samples. Raman measurements with 532 nm laser excitation in the backscattering geometry (Princeton instruments) were also performed. Multiple peaks have been observed in Raman measurements, as shown in Fig. 2(b), which is consistent with the previous study [34,36,48]. Transport measurement was also carried out in our TaSe$_3$ samples. A standard four-terminal connection was used during the high magnetic field measurement with lowest temperature of 0.36 K and largest magnetic field of 38 T carried out in High Magnetic Field Laboratory, Chinese Academy of Sciences. The Hall measurements using a standard Hall-bar configuration was performed in a Physical Property Measurement System (Quantum Design) with lowest temperature of 2 K and largest magnetic field of 9 T. We measured the temperature dependence of resistance of TaSe$_3$ samples, as displayed in Fig. 2(c). The resistance dramatically decreases when cooling down, displaying a metallic behavior with residual resistivity ratio (RRR)$R(300 \text{ K})/R(2 \text{ K}) = 23$, which is similar to the literature [32].

C. Quantum oscillations

We then carried out the magneto-transport measurement of our samples under high magnetic field up to 38 T. Fig. 3(a) displays the field dependence of magneto-resistance (MR) of TaSe$_3$ with the current along the $b$ axis and the applied field along the [1 0 -1] direction at various temperatures from 0.36 K to 78 K. The MR is defined by $[R_{xx}(B) - R_{xx}(0)]/R_{xx}(0) \times 100\%$. It is noticeable that the MR reaches 1800% at 0.36 K and keeps continuously increasing when raising the magnetic field, indicating a non-saturated XMR behavior. In addition, at low temperatures below 10 K, obvious oscillation signals appending on the quadratic background of MR curves
can be observed. In order to further quantitatively analyzing the oscillation behavior, a smooth background was subtracted from the longitudinal resistance $R_{xx}$ and the oscillation patterns as a function of $1/B$ at representative temperatures are presented as seen in Fig. 3(b). One can clearly finds out that the oscillations follow a period proportional to $1/B$, confirming that this is the SdH oscillations caused by the formation of Landau-levels under a high magnetic field.

By fast Fourier transformation (FFT) based on the oscillation components displayed in Fig. 3(b), two major peaks with frequency of $F_\alpha = 99$ T and $F_\beta = 173$ T, which correspond to two oscillation modes, are uncovered, as shown in Fig. 3(c). Thus, there are at least two carrier pockets near the Fermi surfaces contributing to the SdH oscillations in TaSe$_3$, consistent with the prior theoretical [31] and experimental [49] reports that both oscillation modes are associated with the bulk pockets near the Fermi surface. In general, the SdH oscillations can be well described by the Lifshitz-Kosevich (LK) formula [50],

$$\Delta R_{xx} \propto R_T R_D \cos \left[ 2\pi \left( \frac{F}{B} - \frac{1}{2} + \phi \right) \right].$$

The thermal damping factor is $R_T = \frac{\chi}{\sinh (\chi T)}$, and the Dingle damping factor is $R_D = \exp (-\chi T_D)$, where $\chi = \frac{2\pi^2 k_B m^*}{\hbar^2}$. $\phi$ is the phase shift, and $\phi = \frac{\varphi_B}{2\pi} - \delta$, where $\varphi_B$ is the Berry phase and $\delta$ equals 0 and $\pm1/8$ for two-dimensional and three-dimensional systems, respectively. $k_B$ denotes the Boltzmann constant; $\hbar$, the Planck's constant; $F$, the frequency of the oscillation mode; $m^*$, the effective mass. The effective mass $m^*$ can be extracted by fitting the temperature dependence of the corresponding oscillation amplitude to $R_T$, as shown in Fig. 3(d), having $m^*_\alpha = 0.63 m_e$ and $m^*_\beta = 0.75 m_e$. Since there are two oscillation modes in this material, the other related parameters, such as Dingle temperatures, quantum mobilities, etc., need to be extracted by the multiband LK formula [51,52], as depicted in Fig. 3(f). The parameters extracted from the multiband LK fit at 0.36 K, together with the ones
obtained from the analysis of SdH oscillations discussed above, are put in Table I. Specifically, to verify the Berry phase of each oscillation mode, we separate the components from $\alpha$ and $\beta$ modes by FFT filter, and then plot the corresponding Landau fan diagram of each mode respectively in Fig. 3(e). Then we obtain the intercepts at $n$ axis of -0.03 and -0.02, respectively, which are both near to zero, indicating the zero Berry phases. These results are the same as the ones got from LK fitting process as seen in Table I. Note that the ratio $\rho_{xx}/\rho_{xy} \approx 10$ to 100 from Hall measurements under a relatively low field, so the Berry phase derived from the $\rho_{xx}$ could be trustable. The extracted almost zero Berry phases indicate the trivial nature of both the two Fermi pockets contributing to the corresponding two oscillation modes, which indicates that these two Fermi pockets in TaSe$_3$ should belong to bulk pockets rather than the topological surface states. After comparing with the calculated cross-section of each pocket along [1 0 -1] direction displayed in the right panel of Fig. 1(d), we point out that the $\alpha$ oscillation mode corresponds to the hole pocket and the $\beta$ one to electron pockets, further confirming the bulk properties and the zero Berry phase of the two pockets detected in SdH oscillations.

D. Hall measurements

Despite the failure to detect the topological surface states in TaSe$_3$ from SdH quantum oscillations measurements directly, the fascinating non-saturated XMR behavior is observed in this topological insulator candidate, motivating us to exploit the exotic physics of magnetoresistance in this system. As a result, we performed the detailed Hall measurements on this compound under a relatively low field up to 9 T. Fig. 4(a) and 4(b) display the plots of longitudinal resistivity $\rho_{xx}$ and Hall resistivity $\rho_{xy}$ as functions of $B$ at different temperatures ranging from 2 K to 50 K. It is worth noticing that a sign change of $\rho_{xy}$ at low field range from positive to negative occurs when increasing the temperature from 15 K to 50 K (precisely, 20 K to 30 K), suggesting a change of dominant carrier from holes to electrons. Besides, the nonlinear behavior of $\rho_{xy}$ gives the indication for electrical conduction by both electron and hole carriers.
Thus, the Hall response was then further analyzed by the isotropic two-band model, which was usually used to identify the transport contributions from hole-like and electron-like carriers [11,53,54]. The conductivity tensor in this model, is given in a complex representation [3]:

\[
\sigma = e \left( \frac{n_e \mu_e}{1 + i \mu_e B} + \frac{n_h \mu_h}{1 - i \mu_h B} \right). \tag{2}
\]

\( n_e \) (or \( n_h \)) and \( \mu_e \) (or \( \mu_h \)) denote the densities of electrons (or holes) and the mobilities of electrons (or holes), respectively. In order to estimate the carrier densities and mobilities, the longitudinal conductivity \( \sigma_{xx} \) and the Hall conductivity \( \sigma_{xy} \), as shown in Figs. 4(c) and 4(d), can be obtained from a general relation \( \sigma = \rho^{-1} \).

Subsequently, \( \sigma_{xx} \) and \( \sigma_{xy} \) are fitted to the two-band model, where the field dependence of the conductivity tensor \( \sigma_{xx} \) and \( \sigma_{yx} \) are the real and imaginary parts of \( \sigma \) in Eq. (2) [10]:

\[
\sigma_{xx} = \frac{en_e \mu_e}{1 + (\mu_e B)^2} + \frac{en_h \mu_h}{1 + (\mu_h B)^2}, \tag{3}
\]

\[
\sigma_{xy} = -\sigma_{yx} = \left[ \frac{en_e \mu_e^2}{1 + (\mu_e B)^2} - \frac{en_h \mu_h^2}{1 + (\mu_h B)^2} \right]eB. \tag{4}
\]

The results of \( \sigma_{xx} \) and \( \sigma_{xy} \) based on Eqs. (3) and (4) are shown in Figs. 4(c) and 4(d), respectively, plotted in the form of solid curves, exhibiting perfect match except a tiny diverge where field closes zero for \( \sigma_{xx} \). Considering the fact that the Hall signals are more sensitive to the carriers near the Fermi surface, we plot the detailed extracted parameters, densities of carriers \( n_e \) and \( n_h \) and mobilities of carriers \( \mu_e \) and \( \mu_h \), from the two-band model fittings of \( \sigma_{xy} \) as a functions of temperatures from 2 K to 60 K, as shown in Figs. 4(e) and 4(f). Interestingly, we find that the ratio of densities of carriers \( n_h/n_e \), as shown in Fig. 4(e), stays approximately 0.9 when temperature less than 20 K. As the temperature increases above 20 K, the ratio gradually drops and reaches about 0.65 at 60 K. The imperfect but balanced enough ratio of carriers could cause considerable compensation between electrons and holes, which may account for
the non-saturated XMR at low temperature in TaSe₃. In previous theoretical calculations, the ratio of two types of carriers $n_h/n_e \approx 0.9$ can result in a XMR reaching the magnitude of $10^4 \%$ before saturation [2], thus it is understandable to attribute the non-saturated MR behavior to the compensation of two types of carriers. The difference of the magnitude between our data and the theoretical estimation is probably due to the low mobility of carriers [18,55]. In addition, a sudden decrease of densities of both types of carriers as the temperature increases to 30 K appears, suggesting a reconstruction of the Fermi surface, which may be associated with the possible structural phase transition, such as the potential CDW transition reported recently [36].

III. CONCLUSIONS AND PERSPECTIVE

In summary, we carried out systematic investigation on the electronic structure and the corresponding transport behavior for TaSe₃ in this material by combining the first-principles calculations and low-temperature and high-field transport measurements. With the analysis of two-band model, we reveal that the origin of the XMR may be associated with the carrier compensations in TaSe₃. Unfortunately, only bulk properties are detected and the signals from the topological surface states are still concealed. There are a few possible reasons for the absence of the topological surface states signal of TaSe₃ from our experiments. Firstly, there is no real band gap in this system, thus the transport property is dominated by the bulk carriers and the contribution from the surface states may be masked over. Secondly, the calculated topological surface states on (1 0 -1) plane [31], where the field are perpendicular to, is rather subtler than that on (0 1 0) plane and quite lower to the Fermi level, making difficulties to detect. Thirdly, the possible structural phase transition near 30 K may lead to the possibility of the change of Fermi surfaces, so does the topological nature in TaSe₃. Though the smoking gun to experimentally confirm the existence of topological surface states still need to be verified by further studies. our work provides an
opportunity to exploit the interplay between the topology and unsaturated XMR in a topological insulator.

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FIGURE CAPTIONS

Fig. 1. First-principles calculations for TaSe$_3$. (a) The quasi-one-dimensional crystal structure of TaSe$_3$. The blue balls refer to Ta atoms; red ones, Se atoms. (b)-(c) The calculated band structure without (b) and with (c) SOC. (d) Fermi surfaces of TaSe$_3$ (left panel) and its projection on (1 0 -1) plane (right panel). (e) The calculated WCC of six time-reversal invariant momentum planes indicates the topological invariant $Z_2$ = (1; 100). (f) The calculated topological surface states on (0 1 0) plane.

Fig. 2. Characterization of single crystal TaSe$_3$. (a) The EDS spectrum of TaSe$_3$ crystal. The insets show the EDS mapping of Ta and Se, respectively. (b) Raman spectrum of TaSe$_3$ crystal. (c) Temperature dependence of resistance of TaSe$_3$ crystal with RRR = 23.

Fig. 3. XMR and quantum oscillations in single crystal TaSe$_3$. (a) Field dependence of XMR in TaSe$_3$ with the current along the Ta-Ta chains ($b$ axis) and the applied field along the [1 0 -1] direction up to 38 T at selected temperatures. (b) SdH patterns as a function of $1/B$ with the applied field along the $c$ axis at representative temperatures. (c) FFT analysis of $\Delta R_{xx}$. The peaks corresponding to each oscillation mode are marked with Greek letters $\alpha$ and $\beta$. (d) The fits of effective mass for $\alpha$ (99 T) and $\beta$ (173 T) oscillation modes. (e) Landau fan diagram for the SdH oscillations of $\alpha$ and $\beta$ mode with $n$ intercept values -0.03 and -0.02, respectively, indicating the trivial nature of both the hole and the electron pockets. (f) LK fitting of SdH pattern at 0.36 K.

Fig. 4. Two-band model analysis for TaSe$_3$. (a)-(b) Field dependence of Longitudinal
resistivity $\rho_{xx}$ (a) and Hall resistivity $\rho_{xy}$ (b) with field up to 9 T at different temperatures. A negative Hall resistivity appears at 30 K. (c)-(d) Field dependence of $\sigma_{xx}$ (c) and $\sigma_{xy}$ (d) and corresponding two-band model fitting at selected temperatures. (e) Temperature dependence of density of carries $n_e$, $n_h$, and the ratio $n_h/n_e$ extracted from the two-carrier model analysis of $\sigma_{xy}$. The ratio $n_h/n_e$ value stays 0.9 at $T<20$ K and decreases as $T$ increases to 60 K at $T>20$ K. The sudden change of density of carries suggests a reconstruction of the Fermi surface as the temperature goes above 20 K. (f) Carrier mobility $\mu_e$, $\mu_h$ and mobility ratio $\mu_h/\mu_e$ as a function of temperature deducted from the two-carrier model analysis $\sigma_{xy}$. 
**Figures**

(a) [Graphical representation]

(b) [Graphical representation]

(c) [Graphical representation]

(d) [Graphical representation]

(e) [Graphical representation]

(f) [Graphical representation]

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**Fig. 1.** First-principles calculations for TaSe$_3$

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**Fig. 2.** Characterization of single crystal TaSe$_3$. 
Fig. 3. XMR and quantum oscillations in single crystal TaSe$_3$.

Fig. 4. Two-band model analysis for TaSe$_3$. 
Table I. Parameters fitted from SdH oscillations for TaSe$_3$. $F$: oscillation frequency; $S_f$: cross section of the Fermi surface; $k_f$: the Fermi wave vector; $T_D$: the Dingle temperature; $m^*/m_0$: relative effective mass; $\tau$: quantum relaxation time; and $\mu_q$: quantum mobility.

| $F$ (T) | $S_f$ ($10^2\text{Å}^2$) | $k_f$ ($10^2\text{Å}^{-1}$) | $T_D$ (K) | $m^*/m_0$ | $T$ (ps) | $\mu_q$ (cm$^2$V$^{-1}$s$^{-1}$) | Berry phase ($2\pi$) |
|---------|----------------|----------------|-----------|-----------|---------|----------------|---------------------|
| 99      | 0.94           | 5.46           | 5.4       | 0.63      | 0.22    | 614            | 1.01 ± 0.125        |
| 173     | 1.69           | 7.33           | 13        | 0.75      | 0.09    | 211            | 1.12 ± 0.125        |