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Anisotropic Magnetoresistivity in Semimetal $TaSb_2$ *

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We investigate the anisotropic magnetic transports in topological semimetal $TaSb_2$. The compound shows the large magnetoresistance (MR) without saturation and the metal-insulator-like transition no matter whether the magnetic field is parallel to c-axis or a-axis, except that the MR for $\boldsymbol{B}\|c$ is almost twice as large as that of $\boldsymbol{B}\|a$ at low temperatures. The adopted Kohler's rule can be obeyed by the MR at distinct temperatures for $\boldsymbol{B}\|c$, but it is slightly violated as $\boldsymbol{B}\|a$. The angle-dependent MR measurements exhibit the two-fold rotational symmetry below 70 K, consistent with the monoclinic crystal structure of $TaSb_2$. The dumbbell-like picture of angle-dependent MR in $TaSb_2$ suggests a strongly anisotropic Fermi surface at low temperatures. However, it finally loses the two-fold symmetry over 70 K, implying a possible topological phase transition at around the temperature where T_m is related to a metal-insulator-like transition under magnetic fields.

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The study of magnetoresistance (MR) has become one of the most important topics in condense matter physics. The MR not only gives information about the characteristics of the Fermi surface[1] but also is of vital importance to practical applications such as magnetic sensors, magnetic memory and hard drives.[2,3] Generally, a large MR is expected to be discovered in the magnetic materials like multilayer films[4] and Mn-based perovskites,[5] where the large MR originates from the magnetic mechanism. Interestingly, a number of non-magnetic metals have been recently discovered to exhibit the extremely large MR (XMR), such as Cd_3As_2,[6] WTe_2,[7] TaAs-family[8−17] and ZrSiS.[18,19] In comparison with the conventional metals with a small MR of about a few percentages, those materials possess the XMR without saturation at rather high magnetic fields. Several possible mechanisms have been proposed to explain its origin: (1) the linear energy dispersion of Dirac fermions leading to the quantum limit;[20] (2) the compensated electron–hole carrier density;[7,10] and (3) the topological protection mechanism.[21]

Very recently, a new family of topological semimetals (TSMs), the transition-metal dipnictides XPn_2 (X=Ta, Nb, Mo, Pn=P, As, Sb), which crystallize in a centro-symmetry monoclinic structure, have been discovered and investigated.[22−24] The XPn_2-type compounds share some exotic transports such as the XMR and the ultrahigh electronic mobility.[25−28] In particular, the robust low-temperature resistivity plateau and negative MR against the applied magnetic fields,[22,25,29] which are likely attributed to the disentangled bulk electron/hole bands and topological non-trivial surface states,[30] are observed. Following those results, the new members $MoAs_2$ and WP_2 with some common features have been reported by transport measurements.[31,32] Nevertheless, the ARPES experimental results in this family are still of absence and a large number of transports have been mainly focused on the large MR and topological surface state. Thus the anisotropic magnetic transport behaviors related with the Fermi surface structure are highly desirable to be investigated.

In this Letter, we investigate the anisotropic magnetic transports in $TaSb_2$ by measuring its MR at two different crystal directions. The large MR, metal-insulator-transition and robust resistivity plateau are observed when the magnetic field is parallel to c-axis and a-axis. The MR can follow well Kohler's rule for $\boldsymbol{B}\|c$, but it shows weak violation as $\boldsymbol{B}\|a$. The angle-dependent MR (AMR) measurements exhibit the two-fold rotational symmetry below 70 K, consistent with the monoclinic crystal structure of $TaSb_2$. The dumbbell-like picture of AMR in $TaSb_2$ suggests a strongly anisotropic Fermi surface at low temperatures. Though this shape does not change too much below 70 K, the two-fold symmetry finally distorted as T is over 70 K, implying a possible topological phase transition at the characteristic temperature T_m occurring a metal-insulator-like transition under magnetic

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fields.

Single crystals of monoclinic $TaSb_2$ were grown through chemical vapor transport reaction using iodine as transport agent. The detailed synthesis procedures can be found in our previous report.[22] X-ray diffraction patterns were obtained using a D/Max-rA diffractometer with Cu K_α radiation and a graphite monochromator at the room temperature. The single crystal x-ray diffraction determines the crystal grown orientation. The (magneto) resistivity and Hall coefficient measurements were performed using the standard four-terminal method in which the current is parallel to the b-axis. Ohmic contacts were carefully prepared on the crystal with a Hall-bar geometry. Silver wires were attached on the surface of crystals with silver paste. The low contact resistance was obtained after annealing at 573 K for an hour. The physical property was performed in a commercial Quantum Design PPMS-9 system with a torque insert with a temperature range from 2 to 300 K and the magnetic fields up to 9 T.

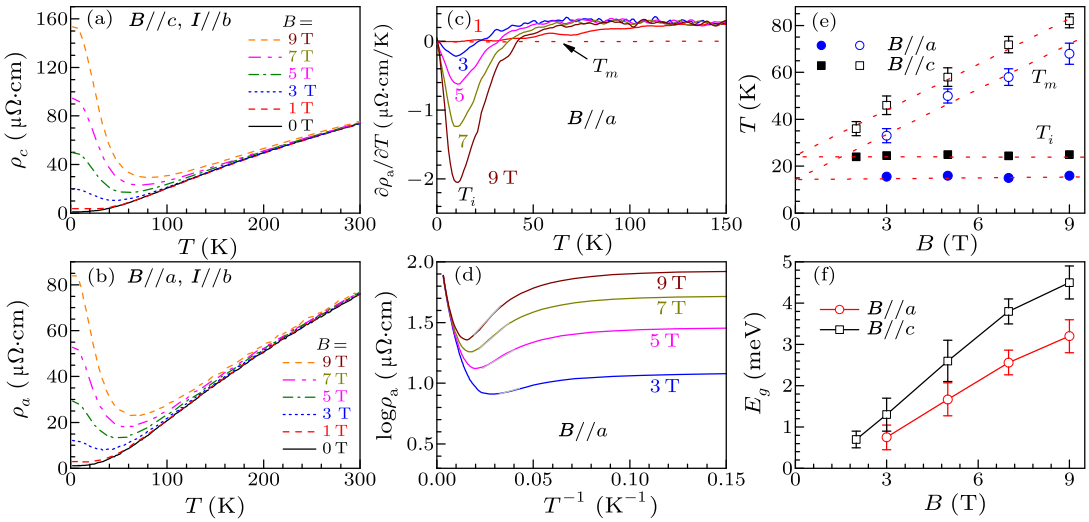

Fig. 1. Temperature dependence of resistivity for $TaSb_2$. Here (a) and (b) show resistivity as a function of temperature in several magnetic fields when $\boldsymbol{B}\|c \perp I$ and $\boldsymbol{B}\|a \perp I$, respectively. (c) Temperature dependence of $\partial\rho/\partial T$ for $\boldsymbol{B}\|a$. (d) The value of $\log(\rho)$ plotted as a function of T^{-1}. The cyan lines show the region of the linear fits. (e) The values of T_m and T_i versus magnetic fields for $\boldsymbol{B}\|a$ and $\boldsymbol{B}\|c$. (f) Field dependence of E_g for $\boldsymbol{B}\|a$ and $\boldsymbol{B}\|c$. The data of $\boldsymbol{B}\|c$ can be found in Ref. [23].

Figure 1 summarizes the magneto-transport properties of $TaSb_2$ with magnetic field along the c-axis and the a-axis. As shown in Figs. 1(a) and 1(b), $\rho(T)$ at zero magnetic field exhibits highly metallic behavior down to 2 K, but sharply increases at low temperatures, followed by a metal-to-insulator-like transition below 70 K when the magnetic field is applied over 3 T. Such behavior has been found in the other known semimetal materials.[7,9] Further cooling temperature, $\rho(T)$ starts to saturate at lower temperature regime, developing a resistivity plateau which has been investigated in our previous work.[22] Notice that increases in $\rho(T)$ for $\boldsymbol{B}\|c$, approaching by two times the values for $\boldsymbol{B}\|a$ at 9 T and 2 K, are observed, suggesting an anisotropic MR in $TaSb_2$.

Figure 1(c) shows the temperature dependence of the derivative $\partial\rho(T)/\partial T$ at different fields for $\boldsymbol{B}\|a$. If we define T_m as the metallic to insulating behavior transition at the one with minimum $\rho(T)$ and T_i as the onset of the plateau, it can be found that the sign change of $\partial\rho(T)/\partial T$ and the drop peak take place at the characteristic temperatures T_m and T_i, respectively, where $\partial\rho(T)/\partial T = 0$ and $\partial^2\rho(T)/\partial T^2 = 0$. As a comparison, the evolution of T_m and T_i versus $\boldsymbol{B}$ for $\boldsymbol{B}\|c$ as well as $\boldsymbol{B}\|a$ is plotted in Fig. 1(e), where T_m increases linearly but T_i remains almost constant with the fields. Such feature implies that the insulating-like behavior is sensitive to the magnetic field while the plateau is robust and intrinsic even at zero field, similar to the case of LaSb.[33] The energy gap of insulator state E_g for $\boldsymbol{B}\|a$ can be obtained by fitting $\rho(T) = \rho_0 \exp(E_\mathrm{g}/K_\mathrm{B}T)$. The result of $\log(\rho)$ as a function of T^{-1} in the range of $T_\mathrm{i} < T < T_\mathrm{m}$ is plotted in Fig. 1(d). The estimated E_g values for $\boldsymbol{B}\|c$ are much larger than that of $\boldsymbol{B}\|a$, as displayed in Fig. 1(f). This large difference further supports the large anisotropic Fermi surface in the sample. The applied magnetic fields can substantially enhance the effective mass of electrons or holes in the Dirac semimetals because of the Zeeman effect. Considering the components of the mobility tensor at the different crystal directions, the increasing resistivity with magnetic fields is expected to be the large difference for $\boldsymbol{B}\|a$ and $\boldsymbol{B}\|c$, resulting in the greatly different energy gaps E_g.

Figure 2 plots the field dependence of the MR below 100 K for $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$ directions, respectively. At 2 K, the resistivity increases sharply with clear Shubnikov-de Haas (SdH) oscillations as the increasing magnetic field is over 6 T in both crystal directions. Warming up temperature results in a decreasing increase in ρ under the magnetic fields. As $T \geq 100$ K,

this curve of ρ versus $\boldsymbol{B}$ becomes flatter, indicative of a small MR at high temperatures. The large positive MR plotted in Figs. 2(c) and 2(d) is observed, reaching about 15000% and 8000% at 2 K and 9 T for $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$, respectively. On heating, the MR decreases monotonously with increasing temperature to 200 K where its MR is several orders of magnitude smaller than the value at 2 K. This very small MR of less than 1% at 200 K and 9 T is in contrast to most of the semimetals with a relatively large MR even at room temperature.[7,16,18,34] This behavior suggests that $TaSb_2$ is the high-metallicity at high temperatures more than others. On the other hand, the MR exhibits the quasi-quadratic for low fields and linear for larger $\boldsymbol{B}$ without saturation, analogous to many known semimetallic materials such as TaAs(P) and WTe_2.[7,9–12]

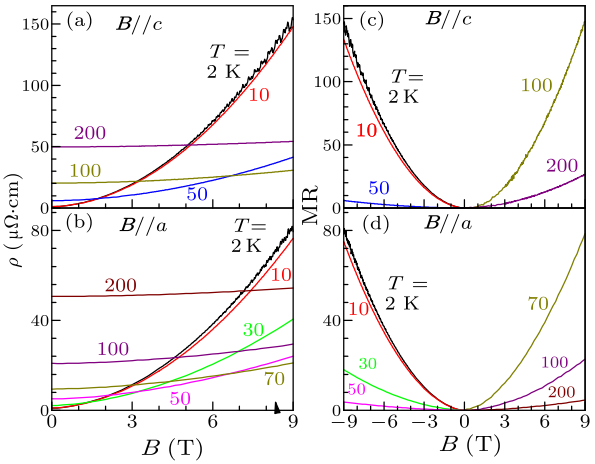

Fig. 2. Magnetic field dependence of (magneto) resistivity in $TaSb_2$. Here (a) and (b) show ρ versus $\boldsymbol{B}$ at different temperatures as $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$, respectively; (c) and (d) display the MR as a function of $\boldsymbol{B}$ for $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$, respectively.

The origin of large MR in some semimetals has been mainly attributed to the electron and hole compensation mechanism.[7,35] In the context, a simplified Kohler's rule: MR $\propto (B/\rho(T,0))^m$, can be adopted to test the MR at distinct temperatures. On the assumption of T-independent carrier density n and the constant effect mass $m*$, the MR at various temperatures can be scaled onto a single line with a constant $m = 1$ and 2 according to this rule. Interestingly, despite the semiclassical origin of this rule, a large number of materials from conventional metals to some quantum matters including a part of topological semimetals can always follow this formula. Here we examine this rule in $TaSb_2$ as shown in Figs. 3(a) and 3(b), and find that it is well obeyed over a wide temperature range for $\boldsymbol{B}\|c$ but this rule is slightly violated as $\boldsymbol{B}\|a$. The obtained m (=1.95) for $\boldsymbol{B}\|c$ is very closed to the classical value 2, while it displays a moderate T-dependent in particular violating the field-square dependence of the MR for $\boldsymbol{B}\|a$, as summarized in the inset of Fig. 3(b). This divergency may be ascribed to the anisotropic Fermi surface topological structure which needs to be further investigated by ARPES measurements.

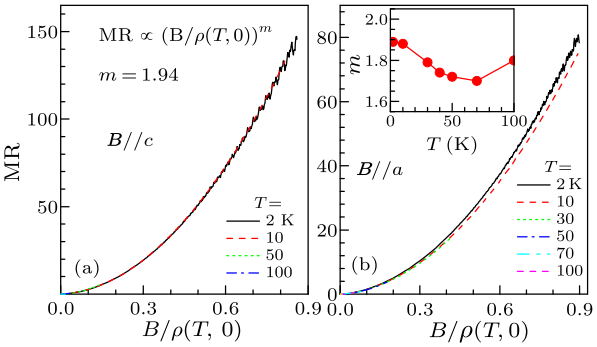

Fig. 3. Kohler's rule in $TaSb_2$. MR versus B/ρ_0 at several temperatures for $\boldsymbol{B}\|c$ (a) and for $\boldsymbol{B}\|a$ (b). The inset shows the fitting m values at several temperatures.

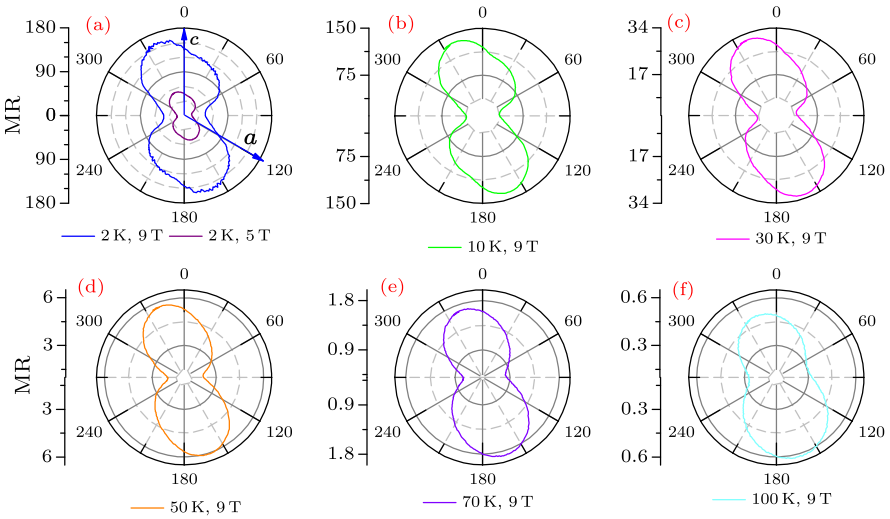

Fig. 4. Angle dependence of MR in $TaSb_2$. (a) AMR at 2 K under two different magnetic fields 5 T and 9 T. (b)–(f) The AMR at different temperatures under 9 T.

Figure 4 shows the transverse MR for the $TaSb_2$ at several distinct temperatures with the rotation of field about b-axis. In Fig. 4(a), the picture of the AMR at 2 K shows a dumbbell-like shape under 5 T and 9 T when the field takes a turn from c-axis towards a-axis, suggesting a strongly anisotropic Fermi surface at low temperatures. Its value first decreases gradually and reaches the minimum (∼4500%) at around $\theta \sim 80°$. With further increasing the angle, the MR starts to increase reversely, displaying a maximum value of 16500% at 9 T at around 165°. The pattern of AMR shows a two-fold rotational symmetry. Both the maximum and the minimum values of MR repeat again for one turn. As $\boldsymbol{B}\|a$ and $\boldsymbol{B}\|c$, the corresponding values in the AMR appear exactly four times and two times, respectively. Those results are highly in agreement with the monoclinic crystal structure of $TaSb_2$. Notice that the position of the maximum and the minimum value does not match the c-axis and a-axis directions of single crystallography, implying a complex Fermi surface topological structure. On heating temperature under a constant field of 9 T, the AMR decreases monotonously, meanwhile the pattern of the dumbbell-like shows the slight change below 50 K, but starts to lose the two-fold rotational symmetry above 70 K, where the characteristic temperature T_m (reported in the previous work[22]) reminds us of the metal to insulator-like transition in resistivity at 9 T. The evolution of the AMR with temperature may be ascribed to a possible topological phase transition, like $MoTe_2$,[35] WTe_2[36,37] and $MoAs_2$.[31]

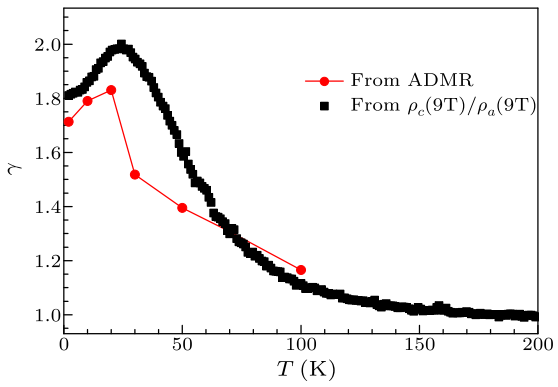

Fig. 5. Temperature dependence of anisotropic value γ.

According to the above investigated experimental results, we can summarize the evolution of temperature dependence of anisotropy value γ (= $\rho_c(9\,\mathrm{T})/\rho_a(9\,\mathrm{T})$) in Fig. 5. We find that at low temperatures the sample exhibits an obviously anisotropic MR (∼ 2). With increasing temperature, the anisotropic value shows a peak at around 20 K, and then decreases sharply to ∼ 1 above 70 K. This temperature-dependent γ suggests that the increase of MR in $\boldsymbol{B}\|c$ is larger than that of in $\boldsymbol{B}\|a$ below 70 K, implying the anisotropic Fermi surface structure in $TaSb_2$. Moreover, the quick increase of γ together with the lost two-fold symmetry below 70 K points to a possible change of Fermi surface topological structure occurring around the temperature.

In summary, we have investigated the anisotropic MR of $TaSb_2$ below 100 K by measuring the MR for $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$ directions, and the AMR below 100 K at 9 T. It is found that the sample shows the unsaturated large MR with linear-dependence at high magnetic fields, the increasing metal-insulator-like transition (T_m) below 70 K and robust resistivity plateau (T_i) with magnetic fields when $\boldsymbol{B}\|c$ and $\boldsymbol{B}\|a$. The MR follows Kohler's rule very well for $\boldsymbol{B}\|c$ but slightly violates this rule as $\boldsymbol{B}\|a$ direction, implying a complex Fermi surface in the present sample. The AMR displays two-fold rotational symmetry below 70 K, consistent with the monoclinic crystal structure of $TaSb_2$. A dumbbell-like picture of AMR in $TaSb_2$ suggests a strongly anisotropic Fermi surface at low temperatures. It gradually changes the shape very weakly but finally loses the two-fold symmetry above 70 K, implying a possible topological phase transition at around the characteristic temperature where T_m undergoes a metal-insulator-like transition under magnetic field.

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