Magnetoresistance and Shubnikov-de Haas oscillation in YSb

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received 4 March 2017; accepted in final form 10 August 2017
published online 7 September 2017

PACS 75.47.-m – Magnetotransport phenomena; materials for magnetotransport
PACS 72.15.Eb – Electrical and thermal conduction in crystalline metals and alloys

Abstract – YSb crystals are grown and the transport properties under magnetic field are measured. The resistivity exhibits metallic behavior under zero magnetic field and the low-temperature resistivity shows a clear upturn once a moderate magnetic field is applied. The upturn is greatly enhanced by increasing magnetic field. At low temperature (2.5 K) and high field (14 T), the transverse magnetoresistance (MR) is quite large ($3.47 \times 10^4 \%$). In addition, the Shubnikov-de Haas (SdH) oscillation has also been observed in YSb. The possible trivial Berry phase extracted from the SdH oscillation, the band structure revealed by angle-resolved photoemission spectroscopy (ARPES) and first-principles calculations demonstrate that YSb is a topologically trivial material. The extremely large MR (XMR) in YSb may originate from the electron-hole compensation.

Introduction. – The magnetoresistance (MR) effect, which describes the change of resistance induced by the magnetic field, is an attractive topic in condensed-matter physics. MR not only has led to many important applications such as magnetic-field sensors, but it also is a useful way to obtain information about the electronic structure of conductors [1,2]. In the past decades, the in-depth study of giant magnetoresistance (GMR) in magnetic multilayers [3,4] and colossal magnetoresistance (CMR) in magnetic oxide materials [5,6] has greatly broadened scientists’ understanding of MR in materials. Recently, much attention has been paid to the XMR around $10^5\%–10^6\%$. The XMR has been detected in several nonmagnetic materials, such as TX ($T = Ta/Nb$, $X = As/P$) [7–15], TX$_2$ ($T = Ta/Nb$, $X = As/Sb$) [16–25], LaX ($X = Sb/Bi$) [26–30], Cd$_3$As$_2$ [31,32], and WTe$_2$ [33–39], etc.

Recently, the rare-earth–based materials LaSb and LaBi with simple rock salt structure have trigged great interest. Both of them exhibit XMR and a resistivity plateau at low temperature and high magnetic field. The transverse MR even reaches $9 \times 10^5\%$ for LaSb at 2 K and 9 T. The SdH oscillation and high mobility have also been observed. However, the origin of the XMR and field-induced transport properties is still controversial. One viewpoint attributes it to the compensation of hole and electron, where the electron-hole balance and high mobility result in the quadratic behavior and very large value of MR [28–30]. The topological protection mechanism is also proposed to explain the XMR, in which the topological protection suppresses backscattering at zero magnetic field and the application of a field will break the protection [31]. Many XMR materials hold nontrivial topological states, which are characterized by a nontrivial Berry phase in transport and band inversion with an odd number of times in ARPES. To reveal the physics underneath, it is greatly needed to find more materials with similar properties.

YSb, which is isostructural to LaSb/LaBi, also exhibits XMR and has received great attention recently [40–42]. As an XMR material, it is necessary to examine the topological property of YSb to clarify the origin of XMR. In this paper, we report the growth of YSb single crystals. The magneto-transport properties of YSb have been studied in detail. YSb exhibits similar field-induced behavior and XMR as LaSb/LaBi. The two major frequencies obtained from the FFT spectra of the SdH quantum oscillation are larger than those in LaSb/LaBi, which reveals a larger cross-sectional area of the Fermi surface in YSb. So, the trivial Berry phase, ARPES results and band structure calculation all demonstrate that YSb is a topologically trivial material. The electron-hole compensation is suggested to be responsible for the XMR in YSb.

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Methods and crystal structure. – Single crystals of YSb were grown with the antimony flux method. The starting elements of Y(99.6%) and Sb(99.5%) were placed into an alumina crucible and sealed in a quartz tube. The quartz tube was put in a high-temperature furnace and heated to 1273 K, held for several hours, then cooled down to 1023 K within 200 hours. At this temperature, the excess Sb flux was removed with a centrifuge. The atomic proportion confirmed by energy dispersive x-ray spectroscopy (EDX) was consistent with 1:1 for Y:Sb. X-ray diffraction (XRD) patterns of single crystal and crushed crystal powder were obtained using a Bruker D8 Advance x-ray diffractometer. TOPAS-4.2 was employed for the refinement. Resistivity measurements were performed with the four-probe method in a physical property measurement system (Quantum Design PPMS-14T). ARPES measurements were performed at the Dreamline beam line of the Shanghai Synchrotron Radiation Facility (SSRF) with a Scienta D80 analyzer. The energy and angular resolutions were set to 15 meV and 0.05, respectively. The samples were cleaved in situ and measured at 30 K in a working vacuum better than 5 × 10^{-11} Torr. The electronic structures of YSb have been studied by using the first-principles calculations. The projector augmented-wave (PAW) method [43,44] as implemented in the VASP package [45–47] was used to describe the core electrons. For the exchange-correlation potential, the modified Becke-Johnson (MBJ) [48,49] exchange potential with the GGA correlation was used. The kinetic energy cutoff of the plane-wave basis was set to be 300 eV. A 20 × 20 × 20 k-point mesh was utilized for the Brillouin zone (BZ) sampling and the Fermi surface was broadened by the Gaussian smearing method with a width of 0.05 eV. Both cell parameters and internal atomic positions were allowed to relax until all forces were smaller than 0.01 eV/Å. The calculated equilibrium lattice constant a is 6.202 Å, which agrees well with the previous experimental value 6.163 Å [50] and the value obtained with x-ray refinement in this paper. Once the equilibrium crystal structures were obtained, the electronic structures were calculated by including the spin orbital coupling (SOC) effect. The Fermi surfaces were studied by using the maximally localized Wannier functions (MLWF) [51,52].

YSb crystallizes in a rock salt structure as shown in fig. 1(a). The XRD pattern of a selected crystal shown in fig. 1(b) indicates that the surface of the crystal is the (0 0 1) plane. The powder XRD pattern of the YSb crystal is shown in fig. 1(c). It was refined using the face-centered cubic structure with space group Fm-3m (No. 225) and the refined lattice parameter a is 6.1628(6) Å, which is in good agreement with the value found from the Inorganic Crystal Structure Database (ICSD). As shown in the photo of fig. 1(b), the typical size of the YSb crystals is about 2 × 2 × 2 mm³.

Results and discussions. – Figure 2(a) plots the temperature dependence of resistivity under several magnetic fields. The electric current is parallel to the (0 0 1) plane and the magnetic field is parallel to the [0 0 1] direction. The temperature-dependent resistivity at zero field exhibits a metallic behavior. When the magnetic field is applied, resistivity decreases with decreasing temperature until a minimum \( T_m \), then it increases until an inflection at \( T_i \) where the resistivity plateau starts to emerge. Figure 2(b) shows the \( \partial \rho/\partial T \) curves derived from fig. 2(a). \( T_m \) is defined as the temperature where the sign changes and \( T_i \) is defined as the temperature where a valley appears. The inset shows \( T_m \) and \( T_i \) as a function of the field, and it is clearly shown that \( T_i \) nearly keeps constant and \( T_m \) nearly increases linearly with increasing field. The behavior which is similar to the metal-to-insulator transition
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Fig. 3: (Color online) (a) Resistivity as a function of the magnetic field in YSb (sample 2, RRR = 63) at several temperatures. Inset: enlarged parts of the resistivity at low temperatures (2.5 K, 3.5 K, 5 K, 6.5 K) under high fields. (b) The logarithmic plot of the MR-H curve at 2.5 K.

at $T_i < T < T_m$ was also observed in previous studies where the mechanism was under debate [34,35,53–55].

Figure 3(a) shows the resistivity of YSb as a function of the field at different temperatures. A clear SdH oscillation was observed at low temperature and high field. The inset shows the enlarged images of oscillating parts. YSb exhibits large transverse MR ($\rho_{xx}(H) - \rho_{xx}(0T)/\rho_{xx}(0T) \times 100\%$) of 3.47% at 2.5 K under the field of 14 T. With the increase of temperature, the transverse MR becomes smaller and the oscillation gradually disappears. The logarithmic plot of the MR-H curve at 2.5 K is shown in fig. 3(b). It shows that the MR follows a semiclassical non-saturating quadratic behavior ($\Delta \rho_{xx} \propto H^m$ with $m \approx 2$). The behavior and origin of the MR will be discussed later.

The oscillation part of resistivity is obtained by subtracting a smooth background. Figure 4(a) plots the oscillation amplitude $\Delta \rho_{xx} = \rho_{xx} - \langle \rho_{xx} \rangle$ of YSb against the reciprocal of the magnetic field at various temperatures. The amplitude displays an obvious periodic behavior and decreases with increasing temperature or decreasing field. The oscillation amplitude can be described by the Lifshitz-Kosevich (L-K) formula [1],

$$\Delta \rho_{xx} \propto \frac{\lambda T}{\sinh(\lambda T_D)} e^{-\lambda T_D} \cos \left[ 2\pi \times \left( \frac{F}{H} - \frac{1}{2} + \beta + \delta \right) \right],$$

where $\lambda = (2\pi^2 k_B m^* / (\hbar e H)), m^*$ is the effective mass of the carrier, and $k_B$ is Boltzmann's constant. $T_D$ and $2\pi/\lambda$ are the Dingle temperature and Berry phase, respectively.

$\delta$ is a phase shift with the value of $\delta = 0$ (or $\pm 1/8$) for a 2D (or 3D) system [56]. Figure 4(b) shows the fast Fourier transform (FFT) spectra. It shows that there exist two principle oscillation frequencies, $F_\alpha = 361$ T and $F_\beta = 780$ T. In the SdH oscillation, the frequency $F$ is proportional to the cross-sectional area $A$ of the Fermi surface normal to the magnetic field, which can be described using the Onsager relation $F = \langle \phi_0 / 2 \pi^2 \rangle A = (\hbar/2 \pi e) A$. These frequencies in YSb are higher than those in LaSb and LaBi [26–29,35], revealing that YSb has larger Fermi surfaces than LaSb and LaBi. In fig. 4(c), we display the temperature dependence of the relative FFT amplitude of frequencies $\alpha$ (main panel) and $\beta$ (inset) of YSb, respectively. The thermal factor $R_T = (\lambda T) / \sinh(\lambda T)$ in the L-K formula has been employed to describe the temperature dependence of the FFT amplitude. The effective masses $m^*_\alpha = 0.17 m_e$ and $m^*_\beta = 0.21 m_e$ can be extracted from the fits. We analyze the main frequency appearing at 361 T to obtain some basic parameters related to the Fermi surface. Considering the circular cross section of the Fermi surface along [0 0 1], the area can be obtained to be $3.45 \times 10^{-2} \text{Å}^2$ by using the Onsager relation. This value is only 3.3% of the whole Brillouin zone in $k_x$-$k_y$ plane taking account of the lattice parameter $a = 6.1628$ Å. The Fermi vector is found to be $0.105 \text{Å}^{-1}$ by using the value of the cross-sectional area. The values of the Fermi velocity and the Fermi
energy are $7.2 \times 10^5$ m/s and 0.502 eV due to the relations $v_F = \hbar k_F/m^*$ and $m^* = E_F/e^2$, respectively. The Dingle temperature $T_D = 17.9 \text{ K}$ is obtained from the slope in the plot of $\ln[D] = \ln[\Delta \rho_2/H \sinh(\Delta T)]$ vs. $1/H$ at $T = 2.5 \text{ K}$ as shown in the inset of fig. 4(c). The corresponding quantum lifetime is $\tau_Q^0 = \hbar/2\pi k_B T_D = 6.8 \times 10^{-14} \text{ s}$. Figure 4(d) shows the $1/H$ curve as a function of the Landau level indices $n$ for the $a$ band. The Berry phase can be extracted based on the Lifshitz–Onsager quantization rule $F/H = n + 1/2 - \beta + \delta$. The peaks and valleys of $\Delta \rho$ at $2.5 \text{ K}$ are denoted as integer and half-integer Landau level indices, respectively. The linear fitting gives a result of $1/2 - \beta + \delta = 0.4679$, indicating a possible trivial Berry phase for the $a$ band. Since the magnetic field is limited to a maximum of $14 \text{ T}$ and the lowest filled Landau level is $n = 27$, which is far from the quantum limit, resistivity measurements under much higher magnetic field are necessary.

Figure 5 shows temperature dependence of the Hall coefficient $R_H = \rho_{xy}/H$ at $14 \text{ T}$ in YSb. $R_H$ in YSb increases sharply at low temperatures and then decreases slowly at high temperatures, which is similar to LaSb. However, YSb shows negative $R_H$ below $40 \text{ K}$ and positive $R_H$ above $40 \text{ K}$ which undergoes a second sign change at $170 \text{ K}$ [27]. The field-dependent Hall coefficient at $2.5 \text{ K}$ is shown in the inset of fig. 5. It shows a clear oscillation, which also indicates the Landau level emptying as the magnetic field increases. The nonlinear behavior of $\rho_{xy}$ indicates the coexistence of electron and hole in YSb. According to the two-band model,

$$\rho_{xy} = \frac{H}{e} \left( n_h \mu_h^2 - n_e \mu_e^2 \right) + \left( n_h - n_e \right) \left( \mu_h \mu_e \right) H^2,$$

where $n_e$ ($n_h$) and $\mu_e$ ($\mu_h$) correspond to electron (hole) concentration and electron (hole) mobility, the curve (the red solid line) is consistent with the experimental curve (the black solid line). At $2.5 \text{ K}$, the concentrations and mobilities obtained from the two-band model are $n_e = 2.06 \times 10^{20} \text{ cm}^{-3}$, $n_h = 1.74 \times 10^{20} \text{ cm}^{-3}$, $\mu_e = 4.02 \times 10^4 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$, and $\mu_h = 0.42 \times 10^4 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$. The similar concentrations suggest the compensation of electron and hole in YSb. However, the ratio $n_h/n_e \approx 0.84$ indicates that the compensation is not perfect.

ARPES measurements were performed to investigate the intrinsic electronic structures of YSb. As illustrated in fig. 6(a), the topology of the Fermi surfaces (FSs) is basically consistent with the previous ARPES [58,59] and calculation [30,60] results on LaSb/LaBi, consisting of two hole pockets at the Brillouin zone (BZ) center and one elliptical electron pocket at the BZ corner. Moreover, we observed some additional FSs around the $\Gamma$-points, which could result from the band folding effect associated with the lattice periodic potential of the termination layer on the (0 0 1) surface. The breaking of the translational symmetry along the $k_z$-direction will result in the shrink of the projection of the bulk BZ on the 2D surface. As compared with the bulk BZ, the projected 2D BZ is reduced by $1/\sqrt{2}$. The FSs at $\overline{\Gamma M}$ ($-\pi, 0, 0$) is folded to $\overline{\Gamma M}$ ($0, -\pi, 0$), leading to the shadow FS around $\overline{\Gamma M}$. The $k_z$ broadening effect may also contribute to the appearance of the folded band structure. The detailed band dispersions along $\overline{\Gamma M}$ are shown in fig. 6(b) and (c), whose momentum location is indicated in fig. 6(a). On moving from $\overline{\Gamma}$ to $\overline{M}$, the outer hole band gradually levels off and then it curves upward, forming a hole band with a maximum at $-0.75 \text{ eV}$ at $\overline{M}$. Additionally, there is a parabolic electron band along $\overline{\Gamma M}$ with a bottom at $-0.30 \text{ eV}$ at $\overline{M}$, forming a band gap of
is employed to describe the resistivity under a magnetic field [31]. The protection strongly suppresses backscattering in zero field and leads to a much longer transport lifetime than the quantum lifetime ($\tau_{\text{tr}}/\tau_{Q} \sim 10^{4}$). In YSb, the transport lifetime is $\tau_{\text{tr}} = \mu_{c} m_{c}^{-3}/e = 3.89 \times 10^{-12}$ s, so the ratio of $\tau_{\text{tr}}/\tau_{Q}$ is about 57. This value is quite small compared with that in Cd$_{3}$As$_{2}$, indicating the lack of topological protection for the $\alpha$ band of YSb. This is also consistent with the topological trivial characteristic of YSb as described above. In the rare-earth-based materials LaSb and LaBi, according to previous works [28–30], the perfect electron-hole compensation and high carrier mobilities naturally explain the XMR based on the two-band model. At the same time, results in another work [27] show that a combination of electron-hole compensation and the mixed $d$-$p$ orbital texture on the electron band plays a key role in determining the magnitude of XMR. In YSb, as revealed by ARPES and first-principles calculations, the gap between yttrium $d$ states (the band shown in yellow in fig. 7) and antimony $p$ states (the band shown in blue in fig. 7) is large and the band inversion is not observed. The absence of the mixture between $d$-orbit and $p$-orbit is clear in YSb. The mixed $d$-$p$ orbital texture may be not suitable to explain the XMR in YSb. Therefore, it is suggested that the XMR in YSb still originates from electron-hole compensation and high mobility of carriers.

**Summary.** – In summary, single crystals of YSb have been grown and the magneto-transport properties have been studied in detail. XMR is observed and the resistivity plateau emerges at low temperature. Moreover, at high magnetic field and low temperature, a clear SdH oscillation appears in YSb. The FFT spectra reveals that there exist two major frequencies in the oscillation and the corresponding effective masses are extracted. The linear fitting in the Landau index plot gives a possible trivial Berry phase. Combining with the electronic structure revealed by ARPES experiments and first-principles calculations, we conclude that YSb is a topologically trivial material. The XMR in YSb can be attributed to electron-hole compensation, and high mobility of carriers.

We thank Z.-Y. Lu, J.-O. Wang and Chen Liu for helpful discussions. This work is supported by the National Natural Science Foundation of China (No. 11574391, No. 11274381), the Fundamental Research Funds for the Central Universities, and the Research Funds of...
Renmin University of China (RUC) (No. 14XNLQ07 and No. 14XNLQ03). Computational resources have been provided by the Physical Laboratory of High Performance Computing at RUC. The Fermi surfaces were prepared with the XCRYSDEN program [61].

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