Extremely large magnetoresistance in the “ordinary” metal ReO$_3$

Qin Chen,$^1$ Zhefeng Lou,$^1$ ShengNan Zhang,$^{2,3}$ Yuxing Zhou,$^1$ Binjie Xu,$^1$ Huancheng Chen,$^1$ Shuijin Chen,$^1$ Jianhua Du,$^4$ Hangdong Wang,$^5$ Jinhu Yang,$^5$ QuanSheng Wu,$^{2,3}$ Oleg V. Yazyev,$^{2,3}$ and Minghu Fang$^{1,6,*}$

$^1$Department of Physics, Zhejiang University, Hangzhou 310027, China
$^2$Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
$^3$National Centre for Computational Design and Discovery of Novel Materials MARVEL, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland
$^4$Department of Applied Physics, China Jiliang University, Hangzhou 310018, China
$^5$Department of Physics, Hangzhou Normal University, Hangzhou 310036, China
$^6$Collaborative Innovation Center of Advanced Microstructure, Nanjing University, Nanjing 210093, China

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The extremely large magnetoresistance (XMR) observed in many topologically nontrivial and trivial semimetals has attracted much attention in relation to its underlying physical mechanism. In this paper, by combining the band structure and Fermi surface (FS) calculations with the Hall resistivity and de Haas-Van Alphen (dHvA) oscillation measurements, we studied the anisotropy of magnetoresistance (MR) of ReO$_3$ with a simple cubic structure, an “ordinary” nonmagnetic metal considered previously. We found that ReO$_3$ exhibits almost all the characteristics of XMR semimetals: the nearly quadratic field dependence of MR, a field-induced upturn in resistivity followed by a plateau at low temperatures, high mobilities of charge carriers. It was found that for magnetic field $H$ applied along the $c$ axis, the MR exhibits an unsaturated $H^{1.75}$ dependence, which was argued to arise from the complete carrier compensation supported by the Hall resistivity measurements. For $H$ applied along the direction of $15^\circ$ relative to the $c$ axis, an unsaturated $H^{1.90}$ dependence of MR up to $9.43 \times 10^4\%$ at 10 K and 9 T was observed, which was explained by the existence of electron open orbits extending along the $k_c$ direction. Two mechanisms responsible for XMR observed usually in the semimetals occur also in the simple metal ReO$_3$ due to its peculiar FS (two closed electron pockets and one open electron pocket), once again indicating that the details of FS topology are a key factor for the observed XMR in materials.

I. INTRODUCTION

The fundamental and applied research on the magnetoresistance (MR) attracted a lot of attention in the past 30 years, due to its applications in magnetic devices for data storage [1–3], magnetic valves [4], magnetic sensors or magnetic switches [2, 5]. The recent discovery of the extremely large magnetoresistance (XMR) up to $10^6\%$ at low temperatures in numerous compounds motivates further research into MR. The list of XMR materials includes both the topologically nontrivial compounds, such as the Dirac semimetals Na$_3$Bi [6] and Cd$_3$As$_2$ [7], Weyl semimetals of TaAs family [8], WTe$_2$ [9], $\beta$-WP$_2$ [10], elemental Ga [11], MoO$_2$ [12] and VA$_2$ [13] as well as topologically trivial semimetals, such as elemental Bi [14], PdCoO$_2$ [15], PtSn$_4$ [16], transition metal dichalcogenides TPn$_2$ (T = Ta and Nb, Pn = P, As and Sb) [17–23], $\alpha$-WP$_2$ [24], rock salt rare earth compound LaBi/Sb$_3$ [25, 26], SiP$_2$ [27] and many others. Although the family of materials showing XMR is expanding, no consistent explanation for the XMR mechanism has been developed so far. Nontrivial band topology inducing linear band dispersion was believed to be responsible for the linear field dependent MR in Cd$_3$As$_2$ [28]. Classical charge-carrier compensation scenario was invoked to explain the non-saturating quadratic MR in WTe$_2$ [9]. Open-orbit trajectories of charge carriers as a result of non-closed Fermi surface (FS) was employed to illustrate the XMR behavior in PdCoO$_2$ [15]. Recently, Zhang et al. [29] studied the transverse MR by combining the FS calculations with the Boltzmann transport theory and the relaxation time approximation, finding that the details of FS topology plays an important role in both the field dependence of MR and its anisotropy.

ReO$_3$ crystallizes in a simple cubic structure with space group $Pm\bar{3}m$ (No. 221). As an “ordinary” nonmagnetic metallic oxide, its calculated band structure and FS [30] compare well with the de Haas-Van Alphen (dHvA) oscillation [31] and optical spectroscopy [32] measurements. The “compressibility-collapse” transition occurring in ReO$_3$ also attracted considerable attention [33–35], especially for the microstructure change at this transition by using nuclear magnetic resonance (NMR) measurements [36], and FS change by using the symmetry analysis [33]. Meanwhile, as a comparison with the copper oxide superconductors exhibiting anomalous resistivity in the normal state, the temperature dependence of the longitudinal resistivity and Hall resistivity of ReO$_3$ was also analyzed [37] by using the Bloch-Grüneisen form as a strong electron-phonon coupling metal.

Usually, in most nonmagnetic metals MR is a relatively weak effect, characterized by a quadratic field dependence at low fields that saturates to a magnitude of a few percent at higher fields, totally different from that in semimetals. In this paper, we measured the longitudinal resistivity, $\rho_{xx}(T,H)$, Hall resistivity, $\rho_{xy}(T,H)$, and...
dependence of MR reaching a large value of $9.43 \times 10^{3}\%$ at 10 K and 9 T, as well as a field-induced up-turn behavior of $\rho_{xx}(T)$, which are the common characteristics for many topologically nontrivial and trivial semimetals.

For magnetic field $H$ applied along the $c$ axis, the MR exhibits a non-saturating $H^{1.75}$ dependence, which we argue arises from the carrier compensation, evidenced by the Hall resistivity measurements. For magnetic field applied along other directions, a similar non-saturating MR dependence with $H^{n}$ ($n = 1.68-1.90$) was observed, which we conclude is due to the existence of electron open orbits extending along the $k_x$ direction. These results indicate that the details of FS topology play an important role in the anisotropy of MR.

II. EXPERIMENTAL AND COMPUTATIONAL METHODS

ReO$_3$ single crystals were grown by a chemical vapor transport method. Polycrystalline ReO$_3$ prepared previously was sealed in an evacuated quartz tube with 10 mg/cm$^2$ TeCl$_4$ as a transport agent, then heated for 2 weeks at 670 K, in a tube furnace with a gradient 30 K. Red crystals with typical dimensions $1.0 \times 1.0 \times 1.0$ mm$^3$ and a (001) easy cleavage plane were obtained at the cold end of the tube. The composition was confirmed to be Re:O = 1:3 by using the energy dispersive x-ray spectrometer (EDXS). The crystal structure was determined using a powder x-ray diffractometer (XRD, Rigaku Gemini A Ultra) with samples produced by grinding pieces of crystals [see Fig. 1(b)]. It was confirmed that ReO$_3$ crystallizes in a cubic structure (space group $Pm\overline{3}m$, No. 221). The lattice parameters $a = b = c = 3.750(2)$ Å were obtained by using the Rietveld refinement to XRD data (weighted profile factor $R_{wp} = 9.62\%$, and the goodness-of-fit $\chi^2 = 2.540$), as shown in Fig. 1(c). Electrical resistivity ($\rho_{xx}$), Hall resistivity ($\rho_{xy}$), and magnetization measurements were carried out by using a Quantum Design physical property measurement system (PPMS - 9 T) or Quantum Design magnetic property measurement system (MPMS - 7 T).

The band structure calculations were performed using the Vienna $ab$ initio simulation package (VASP) [38, 39] with the generalized gradient approximation (GGA) of Perdew, Burke and Ernzerhof (PBE) [40] for the exchange-correlation potential. A cutoff energy of 520 eV and a $13 \times 13 \times 13$ k-point mesh were used to perform the bulk calculations. Magnetoresistance was calculated using the combination of the Boltzmann transport theory and the Fermi surface obtained from first principles [41]. For this purpose we used the WannierTools [42] package, which is based on the maximally localized Wannier function tight-binding model [43–45] constructed by using the Wannier90 [46] package.

Within the relaxation time approximation, the band-wise conductivity tensor $\sigma$ is calculated by solving the Boltzmann equation in presence of an applied magnetic field as [41, 42, 47],

$$\sigma_{ij}^{(n)}(B) = \frac{e^2}{4\pi^2} \int dk \tau_n v_n(k) \overline{v}_n(k) \left( -\frac{\partial f}{\partial \epsilon} \right) \epsilon = \epsilon_n(k),$$  \hspace{1cm} (1)

where $e$ is the electron charge, $n$ is the band index, $\tau_n$ is the relaxation time of $n$th band that is assumed to be independent on the wavevector $k$, $f$ is the Fermi-Dirac distribution, $v_n(k)$ is the velocity defined by the gradient of band energy

$$v_n(k) = \frac{1}{\hbar} \nabla_k \epsilon_n(k),$$ \hspace{1cm} (2)

and $\overline{v}_n(k)$ is the weighted average of velocity over the past history of the charge carrier.

$$\overline{v}_n(k) = \int_{-\infty}^{0} dt e^{\frac{\epsilon}{\tau_n}} v_n(k(t)), \hspace{1cm} (3)$$

The orbital motion of charge carriers in applied magnetic field causes the time evolution of $k_n(t)$, written as,

$$\frac{dk_n(t)}{dt} = -\frac{e}{\hbar} v_n(k(t)) \times B. \hspace{1cm} (4)$$

with $k_n(0) = k$. The total conductivity is the sum of band-wise conductivities, i.e. $\sigma_{ij} = \sum_n \sigma_{ij}^{(n)}$, which is then inverted to obtain the resistivity tensor $\rho = \sigma^{-1}$.

III. RESULTS AND DISCUSSION

As a starting point, we discuss the results of our electronic band structure and FS calculations. Figures 1(i) and 1(j) show the bands without and with considering spin-orbit coupling (SOC), respectively. It is clear the states near the Fermi level ($E_F$) are composed of $d$ orbitals of Re atoms, while $p$ orbitals of O atoms are located at $-2.5$ eV relative to $E_F$, with the SOC resulting only in the separation of the bands near $E_F$. The three pockets of FS of ReO$_3$ are shown in Figs. 1(e)–1(h), respectively, corresponding to the three electron-like surfaces centered at the $\Gamma$ point. The $\alpha$ and $\beta$ pockets are closed, while the $\gamma$ pockets is open along the [100] direction. The $\alpha$ pocket is rather circular in the (100) planes and slightly squared off in the (110) planes, the reverse is true for the $\beta$ pocket. The open $\gamma$ pocket consists of three intersecting cylinders. As discussed in Ref. [30, 33], when magnetic field is applied along [001], two closed extremal orbits exist on the $\gamma$ pocket, as shown in Fig. 1(g). The electron-like orbit labelled $\gamma_1$ occurs on the arms of the cylinder and centered at the X point. The hole-like orbit labelled $\gamma_2$, closed in the extended zone scheme and centered at the M$_2$ point. When magnetic field is applied
along the [111] direction, another extremal open orbit \( \gamma_3 \) exists on the \( \Gamma \) pocket [see Fig. 1(g)]. Because of the nearly degenerate bands along the \( \Gamma-R \) direction [see Fig. 1(d)], the \( \beta \) and \( \gamma \) pockets nearly touch along the [111] direction. The \( \alpha \), \( \beta \) and \( \gamma \) pockets contain 0.093, 0.171 and 0.736 electrons per Re atom, respectively.

In order to study the role of the details of FS topology in the MR, considering the existence of both the closed and open pockets in ReO\( _3 \) mentioned above, we performed experimental measurements of the longitudinal resistivity and the MR anisotropy. Figure 2(a) shows the temperature dependence of the resistivity, \( \rho_{xx}(T) \), measured at both \( \mu_0 H = 0 \) T and 9 T, respectively, with the current applied along the \( a \) axis (\( I \parallel a \)) and magnetic field applied along the \( c \) axis. It is clear that \( \rho_{xx} \) measured at \( \mu_0 H = 0 \) T decreases monotonically with decreasing temperature, \( i.e., \) exhibiting a typical metallic behavior with \( \rho(2 \text{ K}) = 0.02 \mu \Omega \text{ cm} \) and \( \rho(300 \text{ K}) = 6.95 \mu \Omega \text{ cm} \). This corresponds to residual resistivity ratio (RRR) of 348, indicating that our ReO\( _3 \) sample has a relatively high quality, which is consistent with that reported previously [48–50]. Interestingly, \( \rho_{xx}(T) \) measured at \( \mu_0 H = 9 \) T exhibits a behavior similar to that observed in both trivial topologically and nontrivial semimetals [15, 51–55] with a field-induced up-turn in resistivity followed by a plateau at low temperatures, indicating that a large MR indeed emerges in the nonmagnetic metal ReO\( _3 \).

Figure 2(b) shows the angular resistance polar plot \( R_{xx}(H, \theta) \) measured at 2 K in \( \mu_0 H = 3 \) T, 6 T, and 9 T with \( I \) along the \( a \) axis and by rotating the magnetic field \( H \) in the \( b-c \) plane [see the inset of Fig. 2(a)]. The \( R(\theta) \) at 2 K exhibits a nearly fourfold symmetry, \( i.e. \), \( R(\theta) = R(\theta + \pi/2) \), which is consistent with the cubic structure of ReO\( _3 \). An observed minor deviation is probably due to \( I \) not being aligned exactly along the \( a \) axis. The resistance grows quickly from a minimum at \( \theta = 0^\circ \) (\( H \parallel c \) axis) to a maximum at \( \theta = 15^\circ \), and then decreases rapidly to another minimum at \( \theta = 30^\circ \), then increased the second maximum at \( \theta = 45^\circ \). As \( H \) is rotated in the \( \theta = 0 - 90^\circ \) range, the resistance exhibits two maxima of one type (\( \theta = 15^\circ \) and \( 75^\circ \)) and a maximum of another type (\( \theta = 45^\circ \)).

Then, we measured the field dependence of MR, with the conventional definition \( MR = \frac{\Delta \rho}{\rho(0)} = \frac{\rho(H) - \rho(0)}{\rho(0)} \times 100\% \), at 10 K and 20 K, for several chosen magnetic field orientations (\( \theta = 0^\circ, 15^\circ, 30^\circ, 45^\circ \) and \( 60^\circ \)). The results are shown in Figs. 2(c) and 2(d), respectively. For all magnetic field orientations, MR does not show any sign of saturation up to the highest magnetic field 9 T in our PPMS, and exhibits a similar field dependence \( H^0 \) (\( n = 1.68-1.77 \)) for the values of \( \theta = 0^\circ, 30^\circ, 45^\circ \) and \( 60^\circ \). However, for \( \theta = 15^\circ \) we find \( n = 1.90 \), a nearly quadratic scaling with the maximum MR of 9.43 \( \times 10^{3}\% \) at 10 K, 9 T. We note that the field dependence of MR measured at 10 K and 20 K has the same power law for each field.
orientation, indicating that MR can be described by the Kohler scaling law [56]

\[ MR = \frac{\Delta \rho(T, H)}{\rho_0(T)} = \alpha \frac{(H/\rho_0)^m}{\rho_0(T)} . \tag{5} \]

In order to understand the quadratic magnetic field dependence for the $\theta = 15^\circ$ orientation, we plot the representative orbits perpendicular to the magnetic field in Figs. 3(a)–3(d), as well as in Fig. 1(h). The red dashed lines highlight the closed hole orbits, while the green dashed lines indicate the open electron orbits along the $k_x$ direction. Here, the square-shaped red orbits originate from joining the electron pocket fragments in the adjacent periodic replicas of the Brillouin zone (BZ). These are the hole orbits rather than electron orbits. Thus, the non-saturating MR with a quadratic magnetic field dependence ($B^{1.9}$) for the $\theta = 15^\circ$ orientation originates from the existence of open orbits. On the other hand, for the $\theta = 0^\circ$ ($H \parallel c$ axis) orientation, representative orbits perpendicular to the magnetic field are shown in Figs. 4(a)–4(d). The green and red dashed lines indicate the closed electron and hole orbits, respectively, in which the square-shaped red orbits originate from joining the electron pocket (\(\gamma\)) fragments in the adjacent periodic replicas of BZ, i.e., the $\gamma_2$ orbit in Fig. 1(g). In this case, complete compensation of the two kinds of charge carriers can be achieved and confirmed by the Hall resistivity measurements discussed below.

Figure 5 shows the results of our numerical simulations for the resistivity anisotropy and the magnetic field dependence of MR. Figure 5(a) shows calculated anisotropy of resistivity for $H$ rotated in the $b$-$c$ plane, which agrees well with our measurements shown in Fig. 2(b). The angular dependence of MR shows fourfold symmetry caused by the symmetry of crystal structure. The calculated magnetic field dependence of MR also exhibits a subquadratic behavior, i.e., MR scales as $H^{1.9}$ for $\theta = 15^\circ$. All calculated MR results for ReO$_3$ are well consistent with the experimental results discussed above, which indicates that the topology of FS plays the crucial role in defining MR in material.

Figure 6 summarizes resistivity $\rho_{xx}(T, H)$ measured at various temperatures and different magnetic fields with $I \parallel a$ axis, $H \perp (001)$ plane ($\theta = 0^\circ$) in ReO$_3$. The measured resistivity is remarkably enhanced by magnetic field at lower temperatures, and the field-induced upturn is observed. The normalized MR has the same temperature dependence at various fields [see Fig. 6(b)]. Figure 6(c) displays MR as a function of magnetic field at various temperatures, which reaches $4.33 \times 10^{-3}$% at 2 K and 9 T, and does not show any sign of saturation. The MR can be described by the Kohler scaling law [see Fig. 6(d)] with fitting parameters $\alpha = 0.34$ (\(\mu\Omega\) cm/T)$^{1.75}$ and $m = 1.75$. As an “ordinary” nonmagnetic metal, ReO$_3$ exhibits all the common behaviors observed in many trivial or nontrivial topological semimetals [15, 51–55] with XMR, which seems to be unexpected.

In fact, as discussed above, for this particular magnetic field orientation ($\theta = 0^\circ$), there are indeed two kinds of charge carriers in ReO$_3$, evidenced by the nonlinear field dependence of Hall resistivity measured at various temperatures [see Fig. 7(a)]. Following the analysis of $\gamma$-MoTe$_2$ by Zhou et al. [57], as well as our work on MoO$_2$ [12], we analysed the longitudinal and Hall resistivity data by using the semiclassical two-carrier model. In this model, the conductivity tensor, in its complex representation, which is given by [54]

\[ \sigma = \frac{e n_e \mu_e}{1 + i \mu_e \mu_h} + \frac{e n_h \mu_h}{1 - i \mu_h \mu_e}, \tag{6} \]

where $n_e$ and $n_h$ denote the carrier concentrations, $\mu_e$ and $\mu_h$ denote the mobilities of electrons and holes, respectively. To evaluate the carrier densities and their mobilities, we calculated the Hall conductivity $\sigma_{xy} = -\rho_{xy}/(\rho_{xx}^2 + \rho_{yy}^2)$, and the longitudinal conductivity $\sigma_{xx} = \rho_{xx}/(\rho_{xx}^2 + \rho_{yy}^2)$ by using the original experimental $\rho_{xx}(H)$ and $\rho_{xy}(H)$ data. Then, we fit both $\sigma_{xy}(H)$ and $\sigma_{xx}(H)$ data by using the same fitting parameters and their field dependences given by [57]

\[ \sigma_{xy} = \frac{e \mu_0 H n_h \mu_h^2}{1 + \mu_h^2 \mu_e^2 H^2} - \frac{e \mu_0 H n_e \mu_e^2}{1 + \mu_e^2 \mu_h^2 H^2}, \tag{7} \]
broad range of temperatures confirms the coexistence of the two kinds of charge carriers, similar to that observed in many trivial and topologically nontrivial semimetals \cite{15, 51–55}. This verifies once again the leading role of the details of FS topology played in the magnetotransport.

\[ \sigma_{xx} = \frac{\epsilon n_e \mu_n}{1 + \mu_n^2 \mu_h^2 H^2} + \frac{\epsilon n_h \mu_n}{1 + \mu_n^2 \mu_h^2 H^2}. \]  

Figures 7(c) and 7(d) display the fits of both the $\sigma_{xy}(H)$ and $\sigma_{xx}(H)$ measured at $T = 2$, 40, 60, 80 and 100 K, respectively. The excellent agreement between our experimental data and the two-carrier model over a broad range of temperatures confirms the coexistence of electrons and holes in ReO$_3$. Figure 7(b) shows the $n_e$, $n_h$, $\mu_e$ and $\mu_h$ values obtained by the fitting over the temperature range 2–120 K. It is remarkable that the $n_e$ and $n_h$ values are almost the same below 100 K, as shown in the inset of Fig. 7(b), such as at 2 K, $n_e = 4.04 \times 10^{21}$ cm$^{-3}$, and $n_h = 4.03 \times 10^{21}$ cm$^{-3}$. These results indicate that the MR in ReO$_3$ metal for this particular magnetic field orientation ($H \parallel c$) results indeed from the perfect compensation of the two kinds of charge carriers, similar to that observed in many trivial and topologically nontrivial semimetals \cite{15, 51–55}. This verifies once again the leading role of the details of FS topology played in the magnetotransport.

Finally, in order to obtain additional information on the electronic structure, we measured the dHvA quantum oscillations in the isothermal magnetization, $M(H)$, for the $H \parallel c$ axis up to 7 T. As shown in Fig. 8(a), clear dHvA oscillations in the $M(H)$ curves were observed up to 6.0 K from 3.5 T. After subtracting a smooth background from the $M(H)$ data at each temperature, periodic oscillations are visible in $1/H$, as shown in Fig. 8(b). From the Fourier transform (FT) analysis, we derived three basic frequencies 4167 T ($F_\alpha$), 4908 T ($F_\gamma1$) and 6194 T ($F_\beta$) \cite{Fig. 8(c), which are consistent with the results reported by Schirber et al. \cite{33}. In general, the oscillatory magnetization of a three-dimensional (3D) system can be described by the Lifshitz-Kosevich (LK) for-
FIG. 6. (a) Temperature dependence of longitudinal resistivity $\rho_{xx}(T)$ measured at different magnetic fields for the $H \parallel c$ orientation. (b) Temperature dependence of the MR normalized by its value at 2 K at various magnetic fields. The inset is the MR data as a function of temperature. (c) Field dependence of MR of ReO$_3$ at various temperatures. (d) MR as a function of $H/\rho_{xx}(0)$ plotted on a log scale.

FIG. 7. (a) Field dependence of Hall resistivity $\rho_{xy}$ measured for $H \parallel c$ axis at different temperatures. (b) Charge-carrier mobilities, $\mu_e$ and $\mu_h$, and (inset) carrier concentrations, $n_e$ and $n_h$, as a function of temperature extracted from the two-carrier model. Components of the conductivity tensor, $\sigma_{xx}$ and $\sigma_{xy}$, shown in panels (c) and (d), respectively, as functions of magnetic field for temperatures ranging from 2 to 100 K. Dots represent experimental data and red solid lines the fitting curves based on the two-carrier model.

FIG. 8. (a) Magnetization as a function of field measured at various temperatures. (b) The amplitude of dHvA oscillations plotted as a function of $1/\mu_0 H$. (c) Fourier transform (FT) spectra of the dHvA oscillations measured between 1.8 K and 6.0 K. (d) Temperature dependence of relative FT amplitudes for each frequency and the fitting results by $R_T$. (e) The fitting of dHvA oscillations at 1.8 K by the multi-band LK formula. (f) Landau-level indices fan diagram for the three filtered waves of the three frequencies (inset).

The authors calculate the dHvA oscillations amplitude as

$$\Delta M \propto -B^{1/2} R_T R_D R_S \sin[2\pi(F/B - \gamma - \delta)],$$

where $\Delta M$ is the oscillation amplitude, $B$ is the magnetic field, $F$ is the frequency, and $\gamma$ is the phase angle. The authors use this formula to fit the experimental data and determine the effective mass $m^*$, which is related to the electron mass $m_0$ by

$$m^* = \left(\frac{2\pi^2 \hbar^2 m_0}{\alpha}\right).$$

The phase factor $\delta$ is $1/8$ or $-1/8$ for three-dimensional systems. The effective mass $m^*$ can be obtained by fitting the temperature dependence of the oscillation amplitude $R_T(T)$, as shown in Fig. 8(d). For
$F _ { o } = 4167 \, \text{T}$, $F _ { \gamma _ { 1 } } = 4908 \, \text{T}$ and $F _ { \beta } = 6194 \, \text{T}$, the obtained $m ^ *$ are 0.42$m _ { 0 }$, 0.45$m _ { 0 }$ and 0.54$m _ { 0 }$, respectively, somewhat smaller than the calculated values by Schirber et al. [33]. Using the fitted $m ^ *$ as a known parameter, we can further fit the oscillation patterns at given temperatures [e.g. $T = 1.8 \, \text{K}$, see Fig. 8(e)] to the LK formula with three frequencies, from which quantum mobility and the Berry phase can be extracted. The fitted Dingle temperatures $T _ { D }$ are 11.99 K, 11.48 K and 9.00 K, which corresponds to the quantum relaxation times $\tau _ { q } = h/(2 \pi k _ { B } T _ { D } )$ of 0.10 ps, 0.10 ps and 0.13 ps, respectively. The quantum mobilities $\mu _ { q } (\sigma /e m ^ * )$ are 419 cm$^2$/V s, 391 cm$^2$/V s, 423 cm$^2$/V s for $F _ { o }$, $F _ { \gamma _ { 1 } }$ and $F _ { \beta }$, respectively, as listed in Table I. The LK fit also yields a phase factor $- \gamma - \delta$ of $- 0.64 \, (F _ { o } )$, from which the Berry phase $\varphi _ { B }$ is determined to be $1.97 \pi$ for $\delta = 1/8$ and $1.4 \pi$ for $\delta = - 1/8$. The phase factor for $F _ { \gamma _ { 1 } }$ is 0.38, with $\varphi _ { B }$ of 0.01$\pi$ ($\delta = 1/8$) and 1.51$\pi$ ($\delta = - 1/8$). Other results are displayed in Table I.

Similar Berry phase values can also be obtained from the commonly used Landau level fan diagram [61] (i.e. the LL index $n$ as a function of the inverse of magnetic field $1/B_x$). According to customary practice, the integer LL indices $n$ should be assigned when the Fermi level lies between two adjacent LLs [62], where the density of states (DOS) near the Fermi level ($E _ { F }$) reaches a minimum. Given that the oscillatory magnetic susceptibility is proportional to the oscillatory DOS ($E _ { F }$) [i.e. $\Delta (dM/dB) \propto \Delta \text{DOS}(E _ { F } )$] and that the minima of $\Delta M$ and $d(\Delta M)/dB$ are shifted by $\pi /2$, the minima of $\Delta M$ should be assigned to $n - 1/4$. The established LL fan diagram based on this definition is shown in Fig. 8(f). The extrapolation of the linear fit in the fan diagram yields an intercept $n _ { 0 } = 0.81$, which appears to correspond to a Berry phase of $\varphi _ { B } = 2\pi (0.81 + \delta )$, that is $1.87 \pi$ ($\delta = 1/8$) and $1.35 \pi$ ($\delta = - 1/8$) for the $F _ { o }$ band. These results are consistent with the results of the LK formula. Besides, we also obtained the Berry phase for the $F _ { \gamma _ { 1 } }$ band and $F _ { \beta }$ band as listed in Table I. It is well known that topologically non-trivial materials requires a non-trivial $\pi$ Berry phase, while for the trivial materials, the Berry phase equals 0 or $2\pi$. In our sample, the Berry phase is away from the $\pi$, hence we conclude ReO$_3$ is a topologically trivial material.

### IV. SUMMARY

In summary, for successfully synthesized ReO$_3$ crystals, we measured $\rho _ { xx } (T, H)$, Hall resistivity, $\rho _ { xy } (T, H)$, and dHvA oscillations, as well as calculated the electronic band structure and FS to study the anisotropy of MR. It was found that for magnetic field applied along the $c$ axis, the MR exhibits a non-saturating $H^{1.75}$ dependence, which arises from the carrier compensation as supported by the $\rho _ { xy } (T, H)$ measurements. For $H$ oriented along other directions, a similar non-saturating $H^n \, (n = 1.68-1.90)$ dependence of MR was observed, but in this case it stems from the existence of open orbits extending along the $k_x$ direction. As an “ordinary” metal, ReO$_3$ exhibits all the characteristics of XMR semimetals, which is attributed to its peculiar FS, implying the details of FS topology being the key factor underlying the observed XMR in materials.

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*Corresponding author: mhfang@zju.edu.cn

[1] Y. Moritomo, A. Asamitsu, H. Kuwahara, and Y. Tokura, Nature 380, 141 (1996).
[2] J. E. Lenz, Proc. IEEE 78, 973 (1990).
[3] J. Daughton, J. Magn. Magn. Mater. 192, 334 (1999).
[4] S. Wolf, D. Awschalom, R. Buhrman, J. Daughton, v. S. von Molnár, M. Roukes, A. Y. Chetelkanova, and D. Treger, science 294, 1488 (2001).
[5] J. Jankowski, S. El-Ahmar, and M. Oszwaldowski, Sensors 11, 876 (2011).

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### Table I. The parameters obtained by fitting the dHvA data for ReO$_3$.

| Parameters | $F _ { o }$ (LK) | $F _ { \gamma _ { 1 } }$ (LK) | $F _ { \beta }$ (LK) |
|------------|----------------|----------------|----------------|
| Frequency ($T$) | 4167 | 4908 | 6194 |
| $m ^ * / m _ { 0 }$ | 0.42 | 0.45 | 0.54 |
| $T _ { D }$ (K) | 11.99 | 11.48 | 9.00 |
| $\tau _ { q }$ (ps) | 0.10 | 0.10 | 0.13 |
| $\mu _ { q }$ (cm$^2$/V s) | 419 | 391 | 423 |
| $\varphi _ { B } (\delta = + 1/8)$ | $1.97 \pi$ | 0.01$\pi$ | 0.33$\pi$ |
| $\varphi _ { B } (\delta = - 1/8)$ | $1.47 \pi$ | 1.51$\pi$ | 1.83$\pi$ |
| Parameters | $F _ { o }$ (LL) | $F _ { \gamma _ { 1 } }$ (LL) | $F _ { \beta }$ (LL) |
|------------|----------------|----------------|----------------|
| $\varphi _ { B } (\delta = + 1/8)$ | $1.87 \pi$ | 0.97$\pi$ | -0.03$\pi$ |
| $\varphi _ { B } (\delta = - 1/8)$ | $1.35 \pi$ | 0.29$\pi$ | 1.47$\pi$ |

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[59] D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge, 1984).

[60] G. Mikitik and Y. V. Sharlai, Phys. Rev. Lett. **82**, 2147 (1999).

[61] J. Hu, Z. Tang, J. Liu, Y. Zhu, J. Wei, and Z. Mao, Phys. Rev. B **96**, 045127 (2017).

[62] J. Xiong, Y. Luo, Y. Khoo, S. Jia, R. J. Cava, and N. P. Ong, Phys. Rev. B **86**, 045314 (2012).