Extreme magnetoresistance and pressure-induced superconductivity in the topological semimetal candidate YBi

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DOI: 10.1103/PhysRevB.99.024110

(Received 11 October 2018; published 25 January 2019)

Superconductivity in topological materials, either at ambient or extreme conditions, has continued to intrigue scientists as a promising candidate for realizing topological superconductivity, a platform to host the long-sought Majorana fermions in condensed matter. The recent discovery of extremely large magnetoresistance (XMR) in the rare-earth monopnictides opens a new avenue to search for topologically nontrivial states therein, although contrasting opinions argue that it is the carrier compensation effect that is responsible for the observed large, nonsaturating magnetoresistance. Here we study the quantum oscillations and pressure-induced superconductivity in the topologically nontrivial candidate YBi. While the magnetotransport and quantum oscillations do reveal nearly compensated charge carriers, first-principles calculations clearly show that the electronic surface states manifest topologically nontrivial features. Upon applying external hydrostatic pressures, the magnetoresistance is found to decrease and at $P \sim 2.5$ GPa, superconductivity emerges. There exists, however, a regime where XMR and superconductivity coexist in the phase diagram. YBi may therefore represent a rare system for studying the interplay between XMR, topological states, and superconductivity.

I. INTRODUCTION

The recent discovery of extremely large magnetoresistance (XMR) in nonmagnetic semimetals has stimulated tremendous interest in understanding its underlying physical mechanisms and exploring its applications in electronics [1–3]. Among all candidate mechanisms for this XMR, two scenarios represent arguably the most prevalent explanations for these novel phenomena: One scenario argues that the topological states, which forbid the back-scattering of electrons and result in a small residual resistivity in zero field, are not protected in a magnetic field thus increasing its resistivity by orders of magnitude in response to the field. The XMR observed in Dirac semimetals $\text{Na}_3\text{Bi}$ [4], $\text{Cd}_3\text{As}_2$ [5], $\text{ZrTe}_5$ [6], Weyl semimetals TaAs [7], NbAs [8], NbP [9], WTe$_2$ [10], MoTe$_2$ [11], and topological nodal line semimetals PtSn$_4$ [12–14], PdSn$_4$ [15,16] seem to belong to this category. The second explanation attributes the nonsaturating XMR entirely to the classical picture of perfect electron-hole compensation, without invoking the topologically nontrivial states. More recent findings of XMR in lanthanum and yttrium monopnictides $RX$ ($R =$ Lax, Y; $X =$ P, As, Sb, Bi) appear to garner more support for the latter picture, albeit conflicting viewpoints remain [17–26].

Superconductivity may be tuned in topologically nontrivial materials, either through chemical doping or by external pressure. The superconductors achieved in this way are thus regarded as strong candidates of topological superconductivity in which the Majorana fermions exist at the edge or in the vortex center [27,28]. The manipulation of the Majorana fermions may provide the basis for future quantum computing. To date, pressure-induced superconductivity was observed in the quasi-one-dimensional topological insulator $\beta$-Bi$_4$I$_4$ [29], the topological insulator Bi$_2$Te$_3$ [30], the Dirac semimetal HfTe$_5$ [31], and the Weyl semimetal WTe$_2$ [32]. Surprisingly, the pressure-induced superconductivity in these topological semimetals is usually accompanied by the strong suppression or complete destruction of the XMR, casting doubt on the antagonistic interplay between XMR and superconductivity [33,34].

In this article, we report the high-field quantum oscillations and pressure-induced superconductivity in the XMR compound YBi. The magnetotransport and quantum oscillations suggest nearly perfect electron-hole compensation in this material. The first-principle calculations further reveal topologically nontrivial surface states therein. Strikingly, superconductivity ($T_c \approx 5$ K) is observed when pressurizing the
samples to $P \gtrsim 2.5$ GPa. In contrast to other XMR semimetals where superconductivity sets in only when XMR is severely suppressed, superconductivity coexists with XMR in the phase diagram of YBi. Hence, YBi may provide a rare platform to investigate the relationship between XMR, topology, and superconductivity.

### II. EXPERIMENT

Single crystals of YBi were synthesized from the bismuth self flux. Starting materials of yttrium pellets were melted in an electric arc furnace first, so as to minimize the oxidation of the surface layer. Then accurately weighed amounts of high purity yttrium and bismuth elements with the atomic ratio of 11 : 89 (for a total of about 10 g in mass) were mixed thoroughly in a glovebox before being loaded into a quartz tube. The quartz tube was evacuated, sealed, and heated up to 1273 K in a sintering furnace, held at this temperature for one day, and cooled down to 873 K at a rate of 2 K/h. The excess amount of Bi was centrifuged off at this temperature. Finally, high-quality single crystals of YBi of typical dimensions $2.5 \text{ mm} \times 2.5 \text{ mm} \times 2.5 \text{ mm}$ were harvested. Note that the as-grown samples are rather sensitive to air, so extra prudence needs to be taken for the measurements.

The structure of the crystals was analyzed by x-ray diffraction (XRD) using a Rigaku diffractometer with Cu $K\alpha$ radiation and a graphite monochromator at room temperature. The actual stoichiometry of the samples was determined by energy-dispersive x-ray (EDX) spectrometry. Electrical transport properties, i.e., resistivity, magnetoresistance, and the Hall effect, were performed in a PPMS-9 system using the standard four-wire method. Electrical transport in high magnetic fields up to 35 T was carried out at the High Field Magnet Laboratory in Nijmegen. The magnetization was measured by using a MPMS-7 system. For high-pressure measurements, a commercial piston-type cell from Quantum Design was used, and Dephne 7373 oil was used as the pressure-transmission medium.

Electronic-structure calculations with high accuracy were performed by using the full-potential linearized augmented plane wave (FP-LAPW) method implemented in the WIEN2K code. The generalized gradient approximation (GGA) [35] was applied to the exchange-correlation potential calculation. The muffin-tin radii were chosen to be 2.5 a.u. for both Y and Bi atoms. The plane-wave cutoff was defined by $R K_{\text{max}} = 7.0$, where $R$ is the minimum LAPW sphere radius and $K_{\text{max}}$ is the plane-wave-vector cutoff. The self-consistent calculation was performed over a $10 \times 10 \times 10 \times k$-point mesh. The Fermi-surface calculations used a dense $47 \times 47 \times 47$ mesh. To obtain surface state properties, a tight-binding model based on maximally localized Wannier functions [36] was constructed to reproduce the bulk band structure including spin-orbit coupling with Y $s$ and $d$, Bi $s$ and $p$ orbitals. Fermi surfaces and surface state spectra of the (001) surface for each phase were calculated with the surface Green’s function methods as implemented in WANNIERTOOLS [37].

### III. RESULTS

YBi crystallizes in the simple rock-salt structure (space group $Fm\overline{3}m$, No. 225) as illustrated in Fig. 1(e). Figure 1(a) shows the scanning electron microscope (SEM) image of the single crystals of YBi grown in this study which usually show flat facets. The chemical off-stoichiometry was found to be
very small from multiple-spot scanning on the surface with an incident beam energy of 20 keV. A representative example of EDX is shown in Fig. 1(b). The single crystal XRD displays sharp diffraction peaks [Fig. 1(c)], indicating the good quality of the samples and the powder XRD patterns in Fig. 1(d) show no alien phase and all peaks can be well indexed into its face-centered cubic structure. Figure 1(f) shows the Fermi surface of YBi, which will be discussed later. Further sample characterizations can be found in the Supplemental Material (SM) [38] and we also refer the interested readers to the references therein [24,39–50].

The electrical transport properties up to 9 T were presented in the SM [38], which reveal the near-perfect compensation of electrons and holes and are mostly in accord with what was reported by Pavlosiuk et al. [39]. Moreover, de Haas–van Alphen (dHvA) oscillations are clearly seen in a field as low as 4 T. For more information on dHvA oscillations, see Fig. S2b, we extended our measurements to high fields up to 35 T. As weak Shubnikov–de Haas (SdH) oscillations are already discernible from Fig. S2b, we performed a detailed angle-dependent study of the Fermi surface, which is will be discussed later. Further sample characterizations can be found in the Supplemental Material (SM) [38] and we also refer the interested readers to the references therein [24,39–50].

Lifshitz–Kosevich (LK) formula [51,52]:

\[
\Delta \rho \propto R_T R_D R_S \cos \left[ 2\pi \left( \frac{F}{B} + \frac{1}{2} - \frac{\varphi_B}{2\pi} - \delta \right) \right].
\]

(1)

where \( R_T \), \( R_D \), and \( R_S \) are the thermal damping factor, Dingle damping term, and a spin-related damping term, respectively:

\[
R_T = \frac{X}{\sinh (X)}, \quad X = \frac{2\pi^2 T k_B m^*}{eB},
\]

(2)

\[
R_D = \exp \left( \frac{2\pi^2 k_B T D m^*}{eB} \right), \quad R_S = \cos \left( \frac{\pi g_m^*}{2m_e} \right).
\]

(3)

Herein, \( k_B \) is the Boltzmann factor, \( m^* \) is the effective mass, \( m_e \) is the free-electron mass, \( T_D \) is the Dingle temperature, and \( g \) is the Landé g factor. \( \varphi_B \) in Eq. (1) is the Berry phase, and \( \delta \) is an additional phase shift determined by the dimensionality of the Fermi surface, which is \( \delta = 0 \) (\( \delta = \pm 1/8 \)) for two-dimensional (2D) [three-dimensional (3D)] Fermi surfaces. To obtain the effective mass \( m^* \) for each orbit, the temperature dependence of the normalized oscillation amplitude is fit to the Lifshitz–Kosevich formula [Eq. (2)] in Fig. 2(c). The best fits yield \( m^* \) of 0.35\( m_e \), 0.51\( m_e \), 0.68\( m_e \) for the orbits \( \alpha, \alpha', \gamma \), respectively. Because the frequency \( \beta \) is very close to the frequency \( 2\alpha \), we fit the amplitude of frequency \( 2\beta \) instead and obtain \( m^* (2\beta) = 0.45m_e \).

To determine the 3D topology of the Fermi surface, we further performed a detailed angle \( \theta \) dependent study of the magnetoresistance under magnetic-field strengths up to 35 T. Here \( \theta \) is defined as the angle between the magnetic-field and the current-flow direction (along [100]), as schematically shown in the inset of Fig. 2(d). Figures 2(d) and 2(e) show the magnetoresistance under high magnetic field and the oscillatory components (after subtracting the background at \( T = 1.4 \) K), respectively. The oscillation amplitudes diminish
FIG. 3. (a) Temperature dependence of resistivity under different static pressures. The inset highlights the low-temperature regions. (b) MR at $T = 6$ K under different pressures for the sample S1. $\rho/\rho_{6K}$ versus temperature at some selected magnetic fields under (c) 2.6 GPa and (d) 3.0 GPa of S1. $T_c$ is defined as the temperature at which the resistivity starts to drop. (e) Upper critical field $H_{c2}$ of S1 as determined from the panels (c) and (d) and by using the criterion of onset temperature of superconductivity. (f) Pressure dependence of MR at 6 K and 9 T for S1 and S2. (g) Pressure dependence of the resistivity at $T = 6$ K of S1 and S2. (h) Color plot of the zero-field resistivity of S1 on the $T$-$P$ plane.

when the magnetic field is rotated towards [100] direction ($B \parallel I$). As shown in Fig. 2(f), both the FFT frequencies and amplitudes vary with angle. In Fig. 2(g) we compare the experimental frequencies with those from the first-principles calculations. As seen, the calculated frequencies are in reasonable agreement with the experimental data, although notable deviations are also prominent: First, only low frequencies in the $\alpha$ band (below 650 T) are observed, presumably due to the heavier electron masses of the high-frequency orbits. Second, the calculated frequencies for the two hole bands ($\beta$ and $\gamma$ bands) also depart from the experimental values noticeably. While the calculations overestimate the $\beta$ band, the $\gamma$ band frequencies are underestimated. As a result, the total hole concentration is estimated to be similar to that obtained from the first-principles calculations. Third, the $\alpha'$ band shows the distinct angle dependence from that of the calculations.

We also studied the electronic properties of YBi under hydrostatic pressure, with a special focus on the pressure evolution of the XMR. Figure 3(a) shows $\rho(T)$ of one sample (labeled S1) under various applied pressures up to 3.0 GPa. Although previous first-principles calculations predicted that YBi becomes a superconductor with $T_c = 1.29$ K at ambient pressure [53], we have not observed superconductivity down to 1.0 K at 0 GPa [see Fig. 2(a)]. Strikingly however, superconductivity appears at $T_c \approx 5$ K under $P = 2.6$ GPa and $P = 3$ GPa, as shown in the inset of Fig. 3(a). It is worth noting that the residual resistivity under different pressures shows a sudden increase as the sample becomes superconducting [inset of Fig. 3(a)]. This is very similar to what has been observed in the topological nodal line semimetal PbTaSe$_2$, where the residual resistivity shows a discontinuous change under pressure due to a structural transition. The abrupt increase of residual resistivity in the superconducting regime of YBi may also suggest some changes in the electronic ground state. Interestingly, while the resistivity exhibits an abrupt upturn just above $T_c$ at $P = 2.6$ GPa, the resistivity upturn has vanished at $P = 3$ GPa. The reason for the resistivity upturn just above $T_c$ is not clear to us, but very similar behavior has been observed in the bismuth tellurohalide BiTeI [54]. The pressure evolution of the XMR in the normal state at
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FIG. 4. Calculated surface band structures along $\bar{X}-\bar{\Gamma}-\bar{M}-\bar{X}$ [see Fig. 1(f) for the high-symmetry points] of YBi at (a) ambient pressure, and (b) 3 GPa. The bright curves represent the surface states for the (001) surface. (c) Bulk band structures of YBi for ambient pressure (solid lines) and 3 GPa (dotted lines). Three bands cross the Fermi level. The red band consists of Bi $p$ orbital, while the blue band is derived from Y $d$ orbital. (d) Calculated carrier concentrations and the ratio of electron and hole concentrations, $n_\alpha/(n_\beta + n_\gamma)$, as a function of pressure.

Recent ARPES experiments indicate that the XMR semimetal LaSb is topological trivial in nature and its large, nonsaturated MR can be explained by electron-hole compensation [17]. Nevertheless, other ARPES experiments on the same material as well as its sister compound LaBi reveal multiple Dirac cones on their surfaces, although the bulk states look more trivial [18,19]. The observed topological surface states may provide an alternative mechanism for the XMR in this family of rare-earth monopnictides. In YBi, our first-principles calculations shown below explicitly reveal topological surface states that may contribute to the observed XMR, in addition to the electron-hole compensation.

We calculated the bulk and surface electronic structures by using a tight-binding model based on the maximally localized Wannier functions. As shown in Fig. 4(a), at ambient pressure, two nearly degenerate Dirac-cone-like linear surface states at $\bar{X}$ extend to the Fermi energy, above which the degeneracy is lifted. Under 3 GPa, while one Dirac-like dispersion still extends over a large energy range, the other one starts to bend over below the Fermi level and leads to a flat band along $\bar{X}-\bar{M}$, which does not cross the Fermi level. Around the $\bar{\Gamma}$ point ($\bar{\Gamma}-\bar{X}$ direction), at ambient pressure we can also find linear surface states, which become obscured at 3 GPa. Unlike the $\bar{X}$ point, we cannot unambiguously distinguish the surface states at the $\bar{\Gamma}$ point due to the overspreading of convoluted bulk states. Figure 4(c) delineates the bulk band structures under ambient $T = \text{6 K}$ is summarized in Fig. 3(b). As can be seen, the MR shrinks by a factor of two from 23 400% at ambient pressure to 11 500% under $P = 2.6$ GPa, when the superconductivity appears. Nevertheless, even at $P = 3$ GPa, the MR is still very large, reaching a magnitude as high as 7500% at 9 T and 6 K. This is in sharp contrast to many other XMR materials, where the XMR is drastically suppressed or disappears altogether once the superconductivity sets in. As a comparison, in LaBi, the MR reaches a magnitude of order of $\sim 10^6$% at ambient pressure, which reduces to only $\sim 300$% once the superconductivity appears under an applied pressure of 2.6 GPa. A common question arises concerning the nature of the observed superconductivity of YBi under pressure. If it were only the filamentary or surface superconductivity, it would usually be suppressed readily by a magnetic field. We measured the upper critical field at $P = 2.6$ GPa and $P = 3$ GPa by means of temperature sweeps at fixed fields, as shown in Figs. 3(c) and 3(d), respectively. In Figs. 3(c) and 3(d) where we have normalized the resistivity to that at 6 K for clarity, the resistivity upturn just above $T_c$ is progressively suppressed with increasing field. The onset temperature for superconductivity was used to determine $T_c$. The resultant $H_{c2}$ as a function of temperature is plotted in Fig. 3(e), which shows a large $H_{c2}$ compared with its $T_c$. The dataset for another sample S2 is given in the SM [38]. Figures 3(f)–3(h) plot, in sequence, the pressure dependence of MR at 6 K, the pressure dependence of the residual resistivity, and a contour plot of the resistivity in the $T$-$P$ plane. Two distinct background colors highlight the possible electronic structure change at $P \sim 2.5$ GPa.
pressure (solid line) and 3 GPa (dotted line). As seen, a pressure of 3 GPa does not change the bulk band structure significantly. From the orbital weight analysis, the red band consists mainly of the Bi $p$ orbital, while the blue band is primarily derived from the Y $d$ orbital. This particular $d$-$p$ orbital mixing texture, as suggested by Tafti et al. [3], is a generic feature of many topological materials with XMR and is believed to be responsible for the small residual resistivity at zero field and the strong electron scattering in field.

To see how the electron-hole compensation picture evolves with pressure, we also calculated the Fermi surfaces under pressures up to 5 GPa. For all calculated pressures, the Fermi surface consists mainly of the Bi $d$ orbital. This particular band (red band) and two hole pockets ($\beta$ and $\gamma$ bands) located at the center of the Brillouin zone, in a similar fashion to the Fermi surface obtained at ambient pressure [shown in Fig. 1]. A detailed analysis of the Fermi surfaces gives the respective carrier concentration for electrons and holes as a function of pressure, as shown in Fig. 4(d). The ratio of electron and hole concentrations $n_\alpha/(n_\beta + n_\gamma)$ remains close to 1.038 at all pressures, indicating a near-perfect carrier compensation across the pressure range studied. This suggests strongly that electron-hole compensation is the main reason for the observed XMR in YBi. Nevertheless, the surface states which forbid the backscattering of electrons at zero field must also play a role in promoting XMR. In this case, the decrease of MR with pressure (Fig. 3) most likely originates from the change in the electronic structure of the surface states.

**IV. CONCLUSION**

In summary, we report the high-field quantum oscillations and pressure-induced superconductivity in the candidate topological semimetal YBi. Like YSb, LaSb, LaBi, etc., YBi also exhibits XMR behavior and undergoes a magnetic-field-induced metal-insulator-like transition at low temperatures. The analysis of magnetotransport and SdH oscillations indicates nearly compensated charge carriers. However, the first-principles calculations also reveal the presence of topologically nontrivial surface states. Upon tuning the electronic ground state by external pressure, superconductivity appears in a region of the phase diagram in which the XMR coexists. This work may pave the way towards exploring the exotic properties of the topological materials and, potentially, the rich physics arising from the interplay between the topological carriers and the emergent superconductivity.

**ACKNOWLEDGMENTS**

The authors would like to thank C. M. J. Andrew, Zhiqiang Mao, Ali Bangura, and Pabitra Biswas for useful discussions. This work was sponsored by the National Natural Science Foundation of China (Grants No. 11474080, No. U1732162, No. 11504182, No. 11704047, No. U1832147, and No. 11504329). We acknowledge the support of the HFML-RUFOM, member of the European Magnetic Field Laboratory (EMFL). X.X. would also like to acknowledge the financial support from an open program from Wuhan National High Magnetic Field Centre (2015KF15) and six-talent peak of Jiangsu Province (Grant No. 2017-XCL-001). W.H. Jiao was supported from Zhejiang Provincial Natural Science Foundation of China Grant No. LY19A040002.

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