Superconductivity in the nodal-line compound La$_3$Pt$_3$Bi$_4$

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(Dated: April 20, 2022)

Owing to the specific topological states in nodal-line semimetals, novel topological superconductivity is expected to emerge in these systems. In this letter, by combination of the first-principles calculations and resistivity, susceptibility and specific heat measurements, we demonstrate that La$_3$Pt$_3$Bi$_4$ is a topologically nontrivial nodal-ring semimetal protected by the gliding-mirror symmetry even in the presence of spin-orbit coupling. Meanwhile, we discover bulk superconductivity with a transition temperature of ~1.1 K, and an upper critical field of ~0.41 T. These findings demonstrate that La$_3$Pt$_3$Bi$_4$ provides a material platform for studying novel superconductivity in the nodal-ring system.

I. INTRODUCTION

Searching for topological superconductors (TSCs) with Majorana fermions has been one of the hottest topics in contemporary condensed matter physics. The discovery of unconventional superconductivity in the Cu-intercalated Bi$_2$Se$_3$, a topological insulator, has initiated intense interest for TSCs. Although the $p$-wave superconductivity is considered to be an intrinsic TSC, in which the core of the vortex contains a localized quasiparticle with exactly zero energy, the properties of several experimental candidates remain debatable. TSCs can also be realized at the interface of a heterostructure between a strong topological insulator (TI) and an $s$-wave superconductor due to the proximity effect, where the control of the chemical reaction and lattice mismatch at the interface remains challenging. The most promising candidates for TSCs are those in which fully-gapped bulk superconductivity coexists with topologically protected gapless surface/edge states, such as FeTe$_{1-x}$Se$_x$, where the conduction and valence bands touch the Fermi level. Analogous systems (Ln = lanthanoid element, $T = Cu, Au, Rh, Pd, Pt$ and $X = Sb, Bi$) have been reported in the presence of spin-orbit coupling. As a member of Ln$_3$T$_3$X$_4$ family, La$_3$Pt$_3$Bi$_4$ crystallizes in a cubic Y$_3$Au$_3$Sb$_4$-type structure with space group $I43d$ (No. 220), which contains six gliding-mirror symmetry operations. To perform a comparison on the Kondo insulator Ce$_3$Pt$_3$Bi$_4$, measurements of resistivity, magnetic susceptibility, and specific heat of La$_3$Pt$_3$Bi$_4$ above 2 K were performed, and no superconductivity was reported. In this letter, we employed the density functional theory (DFT) to investigate the electronic band structure and its band topology. The results indicate that La$_3$Pt$_3$Bi$_4$ is a topologically nontrivial nodal-ring semimetal. Meanwhile, by performing resistivity, magnetic susceptibility, and specific heat measurements, we discover that La$_3$Pt$_3$Bi$_4$ crystals exhibit bulk superconductivity with a transition temperature $T_c$ ~1.1 K and an upper critical field $\mu_0H_c2(0)$ ~0.41 T. These findings demonstrate that La$_3$Pt$_3$Bi$_4$ provides a material platform for studying novel superconductivity in the nodal-ring system.

II. EXPERIMENTAL AND COMPUTATIONAL METHODS

La$_3$Pt$_3$Bi$_4$ crystals were grown using the method described in Ref. and the crystals with typical dimensions of $0.1 \times 0.1 \times 1$ mm$^3$ were obtained, as shown in the inset of Fig. 1(b). Based on single crystal x-ray diffraction (Rigaku Gemini A Ultra), the crystal structure was confirmed to be a cubic [see Fig. 1(a)], with lattice parameters $a = b = c = 10.175(5)$ Å, which agrees well with the results reported in Ref. Energy-dispersive x-ray spectroscopy measurements were performed using a Zeiss Supra 55 scanning electron microscope to verify the crystal composition of La:Pt:Bi = 3:3:4 [see Fig. 1(b)]. The resistivity, and specific heat
FIG. 1. (Color online) (a) Crystal structure of La$_3$Pt$_3$Bi$_4$ with a Y$_2$Au$_2$Sb$_4$-type structure (SG: I43d); (b) EDX spectrum of a La$_3$Pt$_3$Bi$_4$ single crystal. The inset is a photo of La$_3$Pt$_3$Bi$_4$ crystal; (c) Electronic band structure of La$_3$Pt$_3$Bi$_4$ plotted with orbital characters along high symmetry lines. Red/blue denotes Pt-5$d$ orbitals, and the width of the lines are proportional to the weight of the orbital; (d) Electronic band structure plotted with irreducible representations of the little group along Γ-N and N-P. Along Γ-N, the dark violet (green) lines have eigenvalue of -i (+i) for the gliding-mirror symmetry; while along N-P, the red lines have eigenvalues -1 and -i, gold lines have 1 and -i, dark-green lines have 1 and +i, and blue lines have -1 and +i for the screw and gliding-mirror symmetries, respectively; (e) PDOS of La$_3$Pt$_3$Bi$_4$ in the -5 to 2 eV energy range relative to the Fermi energy; (f) The first Brillouin zone showing the high symmetry points and the nodal ring structure (blue lines) of La$_3$Pt$_3$Bi$_4$. The green circles are the K-path used to calculate the Berry phase.

were measured using a QuantumDesign Physical Properties Measurement System (PPMS-9), with a $^3$He refrigerator attachment down to 0.5 K. The dc magnetization of the crushed powders was measured using a commercial SQUID magnetometer (QuantumDesign MPMS3).

Electronic structure calculations of La$_3$Pt$_3$Bi$_4$ were carried out using plane-wave basis DFT as implemented in the Vienna Abinit Simulation Package (VASP). The valence-ion interactions were approximated using the projected augmented wave method and the exchange-correlation functional was approximated using the Perdew, Burke, and Ernzerhoff flavor of the general gradient approximation. The SOC was considered throughout the calculation as a second variation to the internal stress. The valence-ion interactions were approximated using the WannSymm code. The symmetrization of the resulting Hamiltonian and symmetry analysis of the band structure were performed using the WannierTools code.

III. RESULTS AND DISCUSSION

First, we discuss the electronic band structure and its topological nature based on the DFT calculations. Figures 1(c) and 1(d) show the electronic band structure of La$_3$Pt$_3$Bi$_4$ with SOC. The electronic states near the Fermi level are dominated by the Pt-5$d$Bi-6$p$ orbitals, as shown by the projected density of states (PDOS) in Figure 1(e). The total density of states (DOS) is $n(E_F) = 6.55$ states/(eV·f.u.), or equivalently $\gamma_b = 15.45$ mJ/(mol·K$^2$). By comparing to the experimentally observed value (please refer to the experimental results), we conclude that the electronic correlation is well described at the DFT level. Large SOC splitting is expected and observed in the resulting band structure. Assuming local Ce-4$f$ states, the band structure is similar to that of Ce$_3$Pt$_3$Bi$_4$ at higher temperatures, as expected. At Γ, the highest occupied states are doubly degenerate Γ$_7$, which is extremely close to the Fermi level, and the next highest occupied states are quarter-degenerate Γ$_8$ around $E_F - 70$ meV. All the states in the Γ-N-P plane can be classified using the eigenstates of the gliding-mirror symmetry. The Γ$_7$ state consists of a pair of states with opposite eigenvalues ($\pm i$) of the gliding-mirror symmetry, whereas the Γ$_8$ state consists of two pairs. Meanwhile, at point N, all the states are doubly degenerate because the system preserves the time-reversal symmetry. These two states bear equal eigen-
ues under the gliding-mirror symmetry. Therefore, between \( \Gamma \) and \( N \), an odd number of band crossings must be formed by states with opposite eigenvalues of the gliding-mirror symmetry. A similar argument can also be applied to \( N-P \). Furthermore, since these states can be classified using the gliding-mirror symmetry, they must form a loop in the \( \Gamma-N-P \) gliding-mirror plane. Hence, the DFT band structure calculations show that \( \text{LaPt}_3\text{Bi}_4 \) is a nodal-ring semimetal protected by the gliding-mirror symmetry, as discussed for the isostructure \( \text{CePt}_3\text{Bi}_4 \) at low temperatures.\(^{35} \) The symmetry protected nodal rings in \( \text{CePt}_3\text{Bi}_4 \) are located near \( P \) point; whereas they are located around \( N \) point and \( \Gamma \) point in \( \text{LaPt}_3\text{Bi}_4 \). Such difference is related with partially localized nature of Ce-4f states in \( \text{CePt}_3\text{Bi}_4 \), effectively corresponding to a different electron fillings.

Using the symmetrized tight-binding Hamiltonian obtained with Wannier functions, we identified the nodal ring structure of \( \text{LaPt}_3\text{Bi}_4 \) and calculated the Berry phase around the nodal rings [see Fig. 1(f)]. The nodes of \( \text{LaPt}_3\text{Bi}_4 \) can be generally classified into four sets: 12 symmetrically equivalent small nodal rings around \( \Gamma \) (type-A), 12 symmetrically equivalent large nodal rings across the border of Brillouin zones around \( N \) points (type-B), 12 symmetrically equivalent small nodal rings around \( P \) points, and individual high symmetry nodal points. Among them, only type-B is protected by the crystal symmetries, but are even closer (within 10 meV) to \( E_F \) and large in the \( K \)-space. Therefore, we primarily discuss these two types of nodal rings herein. Using the Wilson loop method, we calculated the Berry phase around both the type-A and type-B nodal rings using the \( K \)-path, as shown by the green circles in Fig. 1(f). Both nodal rings yield Berry phase of \( \pi \), suggesting that both are topologically nontrivial. We note that the bands crossing \( E_F \) lead to 8 Fermi surface sheets (Fig. 2), among which the 4 pockets around \( P \) (panel e of Fig. 2) and 2 pockets around \( H \) (panel a and c of Fig. 2) are not related with the nodal rings. The rest two pockets (panel b and d of Fig. 2) are associated with nodal rings around \( \Gamma \) and \( N \), respectively.

Next, we focus on the discovery of superconductivity in \( \text{LaPt}_3\text{Bi}_4 \). Figure 3(a) shows the temperature dependence of the resistivity between 0.5 and 300 K for a \( \text{LaPt}_3\text{Bi}_4 \) crystal. At \( T = 300 \text{ K} \), the resistivity is about 185 \( \mu \Omega \cdot \text{cm} \). Upon cooling down from 300 K, the resistivity exhibits metallic characteristics with a continuous change in the slope. The residual resistivity ratio \( \frac{\rho(300 \text{ K})}{\rho(2 \text{ K})} \) is about 5, larger than that reported previously,\(^{35} \) indicating the high quality of our crystal. At \( T_{\text{C onset}} \sim 1.1 \text{ K} \), the resistivity starts to drop abruptly; then at \( T_{\text{C onset}} \sim 0.86 \text{ K} \), reaches zero, which is consistent with the onset of a diamagnetic transition [see Fig. 3(b)], indicating the occurrence of a superconducting transition. As shown in the right inset of Fig. 3(a), the temperature dependence of resistivity (\( \leq 20 \text{ K} \)) in the normal state exhibits non-Fermi liquid (NFL) behavior. Since the electronic correlation effect is not so prominent, as evidenced by the comparison between DOS from DFT calculations and \( \gamma \), the origin of such NFL behavior is possibly related with the topological nodal ring structure near \( E_F \). Figure 3(b) presents the temperature dependence of the susceptibility, \( \chi(T) \), below 1.2 K, measured with both zero-field cooling (ZFC) and field cooling (FC) processes. The superconducting volume fraction at \( 0.4 \text{ K} \) is about 37\%, indicating that bulk superconductivity emerges below \( T_C \) in \( \text{LaPt}_3\text{Bi}_4 \). It is worth noting that \( \text{LaPt}_3\text{Bi}_4 \) is the first reported superconductor in

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**FIG. 2.** (Color online) Fermi surface of \( \text{LaPt}_3\text{Bi}_4 \). (a-e): Separated fermi surface sheets. Three of the Fermi surface sheets around \( P \) are too small, so we plot them together in panel (e). (f): Full Fermi surface plot.
the \( \text{La}_3\text{T}_3\text{X}_4 \) (\( \text{Ln} \) = lanthanoid element, \( \text{T} = \text{Cu, Au, Rh, Pd, Pt} \) and \( \text{X} = \text{Sb, Bi} \)) family, implying that other member may be a superconductor as well; however, this must be confirmed through further investigations. We also note that the half-Heusler \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) compound was found to be a non-centrosymmetric superconductor with a \( T_C \) of \( \sim 0.9 \text{ K} \), \( \mu_0H_{c2}(0) = 1.5 \text{ T} \), and another candidate for \( \text{TCS}^{\text{Bi}} \), however, the superconducting properties, such as \( \mu_0H_{c2}(0) \), specific heat jump at \( T_C \), as well as the properties in the normal state, such as the \( \rho(T) \) behavior, differ from those exhibited by \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) reported herein.

Figure 3(c) shows the temperature dependence of the resistivity, \( \rho(T, H) \), around the superconducting transition measured at various magnetic fields applied perpendicular to the current. With increasing magnetic field, the superconducting transition gradually shifts to a lower temperature. We estimated the \( H_{c2} \) using the middle temperature of the superconducting transition \( (T_C)^{\text{mid}} \) and plotted \( H_{c2}(T) \), as shown in the inset of Fig. 3(c). According to the Ginzburg-Landau (GL) theory, \( H_{c2}(T) \) can be fitted using the formula \( H_{c2}(T) = H_{c2}(0)(1 - t^2)/(1 + t^2) \), to get the zero-temperature upper critical field \( \mu_0H_{c2}(0) \approx 0.41 \text{ T} \), where \( t \) is the reduced temperature \( (t = T/T_C) \), as shown by the blue line in the inset of Fig. 3(c). The estimated \( H_{c2}(0) \) is much lower than that of the half-Heusler \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) compound (\( \approx 1.5 \text{ T}^{\text{Bi}} \)). Furthermore, the superconducting coherence length \( \xi_0 \) for the \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) compound was estimated to be \( \sim 28.4 \text{ nm} \) using the formula \( H_{c2}(0) = \Phi_0/2\pi\xi_0^2 \), where \( \Phi_0 \) (\( 2.071 \times 10^{-15} \text{ Wh} \)) is the fluxoid quantum.

To measure the specific heat, \( C(T) \), we arranged several needle-like crystals on the measurement puck. \( C(T)/T \) as a function of \( T^2 \), measured at zero magnetic field, is shown in Fig. 3(d). A significant specific heat jump was observed at approximately 0.8 K, thereby confirming again that \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) exhibits bulk superconductivity. We used the formula \( C/T = \gamma + \beta T^2 \) to fit the \( C(T) \) data (1.1 - 2 K) in the normal state to obtain the Sommerfeld coefficient \( \gamma = 17.3 \text{ mJ/(mol-K}^2) \) and the Debye constant \( \beta = 9.9 \text{ mJ/(mol-K}^4) \), corresponding to the Debye temperature \( \Theta_D = 125 \text{ K} \). The electronic specific heat \( C_{es}(T) \) in the superconducting state was obtained by subtracting the phonon contribution term \( \beta T^3 \) from the total \( C(T) \), as shown in the inset of Fig. 3(d).

Finally, we make a simple analysis of the superconductivity in \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) based on our experimental and calculation results. The electronic specific heat coefficient \( \gamma \) can be related with \( \gamma_b \) via \( \gamma = (1 + \lambda_{ep})\gamma_b \) in weakly correlated materials, where \( \lambda_{ep} \) is the electron-phonon coupling strength. This leads to an estimation of \( \lambda_{ep} \approx 0.12 \) in this material. Such small electron-phonon coupling results in negligible phonon mediated \( T_C \) using BCS formula \( T_C = \Theta_D \exp[-1/(\lambda_{ep} - \mu^*)] \), where \( \Theta_D \) is the Debye temperature, and \( \mu^* \) is the Coulomb repulsion pseudopotential (chosen within the normal range of 0.10 - 0.15). Therefore, despite of its low superconducting \( T_C \), it is highly possible that the pairing mechanism of \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) is unconventional.

IV. CONCLUSIONS

In summary, by combining the first principles calculations and resistivity, susceptibility and specific heat measurements, we discovered bulk superconductivity with \( T_C^{\text{Inset}} = 1.1 \text{ K} \), and \( \mu_0H_{c2}(0) = 0.41 \text{ T} \) in \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) compound. It was confirmed that \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) is a nodal-ring semimetal protected by the gliding-mirror symmetry. These results indicate that \( \text{La}_3\text{Pt}_3\text{Bi}_4 \) provides a material platform for studying novel superconductivity in the nodal-ring system.

ACKNOWLEDGMENTS

This work was supported by the Ministry of Science and Technology of China under Grant No. 2016YFA0300402 and the National Natural Science Foundation of China (NSFC) (Grant Nos. 11974095, 11874137, 12074335, 11874136), and the Fundamental Research Funds for the Central Universities. The calcula-
tions were performed on the High Performance Comput-
ing Cluster of Center of Correlated Matters at Zhejiang
University, and Tianhe-2 Supercomputing Center.

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