Superconductivity in noncentrosymmetric YPtBi under pressure

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We report a high-pressure single-crystal study of the noncentrosymmetric superconductor YPtBi ($T_c = 0.77$ K). Magnetotransport measurements show a weak metallic behavior with a carrier concentration $n \simeq 2.2 \times 10^{19}$ cm^{-3}. Resistivity measurements up to $p = 2.51$ GPa reveal superconductivity is promoted by pressure. The reduced upper critical field $B_{c2}(T)$ curves collapse onto a single curve, with values that exceed the model values for spin-singlet superconductivity. The B_{c2} data point to an odd-parity component in the superconducting order parameter, in accordance with predictions for noncentrosymmetric superconductors.

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I. INTRODUCTION

Recently, superconductivity with a transition temperature $T_c = 0.77$ K was discovered in the noncentrosymmetric half Heusler compound YPtBi.[1] Noncentrosymmetric superconductivity forms a prominent research topic as it offers a wide-ranging, fruitful playground for the investigation of unconventional superconducting phases.[2] The lack of an inversion center in the crystal structure causes an electric field gradient, which creates an antisymmetric Rashba-type spin-orbit coupling. This results in a splitting of the Fermi surface, which thwarts spin-singlet or spin-triplet Cooper pairing of the conventional type. Instead, new pairing states, notably mixed even- and odd-parity Cooper pair states, are predicted to make up the superconducting condensate.[3] The field of noncentrosymmetric superconductors was initiated by the discovery of superconductivity in the heavy-fermion material $CePt_3Si$ ($T_c = 0.75$ K).[4] Other well-documented examples of noncentrosymmetric superconductors are $CeRhSi_3$ ($T_c = 1.1$ K under pressure),[5] $CeIrSi_3$ ($T_c = 1.6$ K under pressure),[6] Li_2Pt_3B ($T_c = 2.6$ K),[7] and Mo_3Al_2C ($T_c = 9.2$ K).[8,9] For several noncentrosymmetric superconductors, solid evidence for an odd-parity component in the superconducting order parameter has been extracted from critical magnetic fields exceeding the spin-singlet Pauli paramagnetic limit and/or line or point nodes in the superconducting gap function.[2]

Yet another motive to investigate YPtBi is provided by electronic band structure calculations.[10,11] First principle calculations carried out on a series of rare earth (RE) ternary half Heusler compounds predicted several of them to have a topologically nontrivial band structure, due to a sizable Γ_6–Γ_8 band inversion. This allows for a classification as a (candidate) three-dimensional (3D) topological insulator. A 3D topological insulator is insulating in the bulk, but has conducting surface states protected by a nontrivial Z_2 topology.[12,13] Notably, the nonmagnetic REPtBi compounds LuPtBi and LaPtBi, as well as YPtBi, are predicted to have a relatively strong band inversion. Transport experiments reveal LuPtBi is metallic,[14] while YPtBi (Refs. 1 and 15) and LaPtBi (Ref. 16) are semimetals that become superconducting [$T_c = 0.9$ K for LaPtBi (Ref. 16)]. The nontrivial topology of the electron bands makes YPtBi and LaPtBi promising candidates for topological superconductivity with protected Majorana surface states.[17] Topological superconductors are rare, and only a few cases are known: the correlated metal Sr_2RuO_4 (Ref. 18), which is conceivably a time-reversal symmetry-breaking chiral two-dimensional (2D) p-wave superconductor,[19] and the intercalated thermoelectric effect material $Cu_xBi_2Se_3$ (Refs. 20–22), for which a time-reversal symmetric, fully gapped, odd-parity superconducting state has been proposed.[23]

YPtBi has a cubic structure and crystallizes in the $F\bar{4}3m$ space group. It was first prepared as non-f electron reference material in the systematic investigation of magnetism and heavy-fermion behavior in the REPtBi series.[15] Magnetotransport measurements carried out on single crystals grown out of Bi flux point to semimetalliclike behavior.[1,15] The resistivity $\rho(T)$ increases steadily upon cooling below 300 K and levels off below $\sim$60 K (Ref. 1). The Hall coefficient R_H is positive and quasilinear in a magnetic field, allowing for an interpretation in a single-band model with hole carriers (Ref. 1). The carrier concentration n_h is low and shows a substantial decrease upon cooling from 2×10^{19} cm^{-3} at 300 K to 2×10^{18} cm^{-3} at 2 K. Concurrently, the Sommerfeld coefficient in the specific heat is very small, $\gamma \leqslant 0.1$ mJ/molK^2 (Ref. 24). YPtBi is diamagnetic and the magnetic susceptibility χ attains a temperature independent value of -10^{-4} emu/mol (Ref. 24).

The transition to the superconducting state takes place at $T_c = 0.77$ K,[1] where the resistivity sharply drops to 0. At the same temperature a diamagnetic screening signal appears in the ac susceptibility χ_{ac}, but the magnetic response is sluggish. The upper critical field $B_{c2}(T)$ shows an unusual quasilinear behavior and attains a value of $\sim$1.5 T for $T \to 0$ K.[1] Heat capacity measurements around the normal-to-superconducting phase transition, which are a standard experimental tool to provide evidence for bulk superconductivity, have not been reported yet. We note that the extremely small γ value makes this a difficult experiment. On the other hand, the confirmation of superconductivity with an identical critical temperature $T_c = 0.77$ K in our single crystals and the observation of a diamagnetic signal in χ_{ac}, which corresponds to a superconducting volume fraction of 30%,[25] point to a bulk superconducting phase.

Here we report the response of the superconducting phase of YPtBi to pressures up to 2.51 GPa. Transport measurements on single crystals confirm superconductivity with a critical temperature $T_c = 0.77$ K. Under pressure superconductivity is enhanced and T_c increases at a linear rate of 0.044 K/GPa. The upper critical field $B_{c2}(T)$ curves taken at different pressures collapse onto a single curve, with values that exceed the model values for spin-singlet superconductivity. The B_{c2} data point to the presence of an odd-parity Cooper pairing component in the superconducting order parameter, in agreement with predictions for noncentrosymmetric and topological superconductors.[3,17,23]

II. EXPERIMENTAL

Several batches of YPtBi were prepared out of Bi flux[26] from a starting composition Y:Pt:Bi = 1:1:1.4. First Pt and Bi were melted together and put with Y in an alumina crucible. The crucible was placed in a quartz tube, which was sealed in an argon atmosphere ($p = 0.3$ bar). The tube was heated slowly and kept at a temperature of 1250 °C for 24 h. The cooling rate was 1 °C/h down to 900 °C. The collected crystals have free-growth planes with sizes up to 4 mm. Electron probe microanalysis confirmed the 1:1:1 ratio. X-ray powder diffraction was used to check the $F\bar{4}3m$ space group. The deduced lattice parameter $a = 6.650$ Å is in good agreement with the literature.[1] Single crystals taken from these batches reproducibly showed superconductivity with a resistive transition at $T_c = 0.77$ K.

The resistivity and Hall effect were measured using a MaglabExa system (Oxford Instruments) for $T = 4$ to 300 K and in a ^{3}He refrigerator (Heliox, Oxford Instruments) for 0.24 to 10 K. Additional $\rho(T)$ data were taken in a dilution refrigerator (Kelvinox, Oxford Instruments) down to $T = 0.04$ K. The transport data were measured using a low-frequency ($f = 16$ Hz) lock-in technique with a low excitation current ($I = 100\ \mu$A). The high-pressure transport measurements were carried out using a hybrid clamp cell made of NiCrAl and CuBe alloys. Samples were mounted on a plug which was placed in a Teflon cylinder with Daphne oil 7373 as the hydrostatic pressure transmitting medium. The pressure cell was attached to the cold plate of the ^{3}He refrigerator. The pressure was determined in situ by the superconducting transition of a Sn specimen.

III. RESULTS

In Fig. 1 we show a typical resistivity trace $\rho(T)$. Upon cooling below 300 K, $\rho(T)$ gradually drops and levels off below 30 K. This demonstrates our YPtBi crystals behave as a metal, rather than as a semimetal.[1,15] The carrier concentration $n_h(T)$ is low and displays a weak temperature variation (Fig. 1). Near room temperature the transport parameters of our samples are quite similar to those reported in Ref. 1: ρ(295 K) equals 230 $\mu\Omega$ cm versus 300 $\mu\Omega$ cm (in Ref. 1) and n_h(295 K) equals 2.2×10^{19} cm^{-3} versus 2×10^{19} cm^{-3} (in Ref. 1). A major difference is found in $n_h(T)$, which is close to temperature independent for our sample, but drops by a factor 10 upon cooling to 2 K in Ref. 1. The origin of the dissimilar transport behavior is unclear. Possibly trapping of carriers at defects upon lowering the temperature causes semimetalliclike behavior in the samples used in Refs. 1 and 15. The metallic behavior is robust under pressure (see the inset in Fig. 1). R(295 K) increases linearly with pressure, resulting in a 20% increase at the maximum pressure of 2.51 GPa. The residual resistance R(4 K) increases at the same rate. The residual resistance ratio, RRR defined as R(295 K)/R(4 K), of our samples amounts to ∼1.4 at $p = 0$. A sharp superconducting transition is observed for all samples at $T_c = 0.77$ K. The width of the transition ΔT_c, as determined between 10 and 90% of the normal state R value, is 0.06 K.

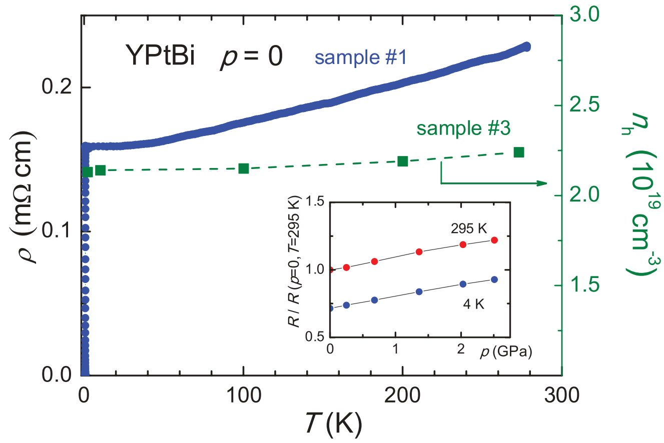

FIG. 1. (Color online) Resistivity (closed circles—left axis) and carrier concentration (closed squares—right axis) of YPtBi as a function of temperature at ambient pressure. Inset: Resistance at 295 and 4 K as a function of pressure. Resistance values are normalized to the room temperature value at ambient pressure, $R(p = 0, T = 295$ K).

The superconducting transition under pressure is shown in Fig. 2. Notice that the $p = 0$ data are taken on a different sample in a separate experiment. T_c, as determined by the maximum in the slope $d\rho/dT$, increases linearly with pressure at a rate of 0.044 K/GPa (see inset in Fig. 2). The width of the transition does not change with pressure, which is indicative of a homogeneously applied pressure. The $\rho(T)$ data taken on sample #2 (under pressure) show a tiny structure just above 1 K. This feature is insensitive to pressure and suppressed by

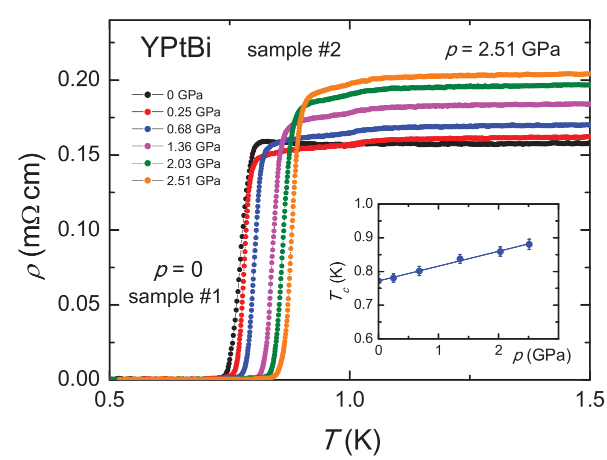

FIG. 2. (Color online) Superconducting transition of YPtBi at pressures of 0, 0.25, 0.68, 1.36, 2.03, and 2.51 GPa (from left to right). Data at $p = 0$ taken on sample #1; data under pressure on sample #2. Inset: Superconducting transition temperature as a function of pressure. The solid line is a linear fit to the data points with slope $dT_c/dp = 0.044$ K/GPa.

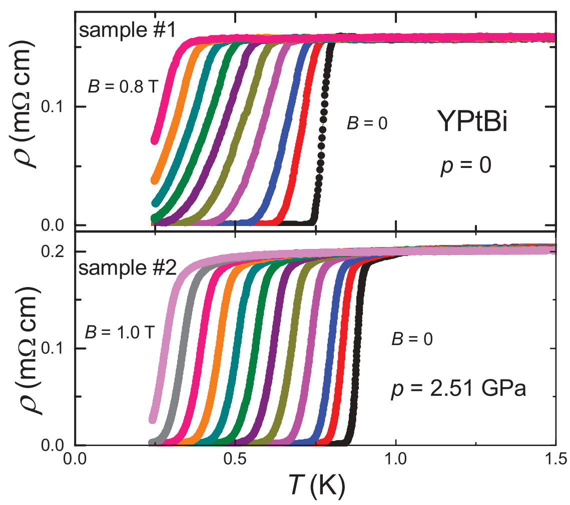

FIG. 3. (Color online) Superconducting transition of YPtBi measured in magnetic fields of 0, 0.05, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, and 1.0 T (from right to left). Upper frame: $p = 0$, sample #1. Lower frame: $p = 2.51$ GPa, sample #2.

a small magnetic field ($B \sim 0.1$ T, see Fig. 3). It has not been observed in other samples.

The depression of superconductivity by a magnetic field was measured in fixed fields up to $p = 2.51$ GPa. Representative data are shown in Fig. 3. For sample #1 measured at $p = 0$, ΔT_c increases almost by a factor 2 to 0.12 K in the highest field. For sample #2, measured under pressure, ΔT_c is virtually pressure and field independent, which attests to its high quality. $T_c(B)$ determined by the maximum in $d\rho/dT$ at fixed B is reported for each pressure in Fig. 4. $B_{c2}(T)$ is dominated by a quasilinear temperature dependence down to $T_c/3$. At temperatures below this, data taken in the dilution refrigerator show $B_{c2}(T)$ curves towards the vertical axis. For $p = 0$ we obtain $B_{c2}(T \to 0) \simeq 1.23$ T. Notice that close to T_c all data sets show a weak curvature or tail. The curvature is less pronounced for the better sample (#2) measured under pressure.

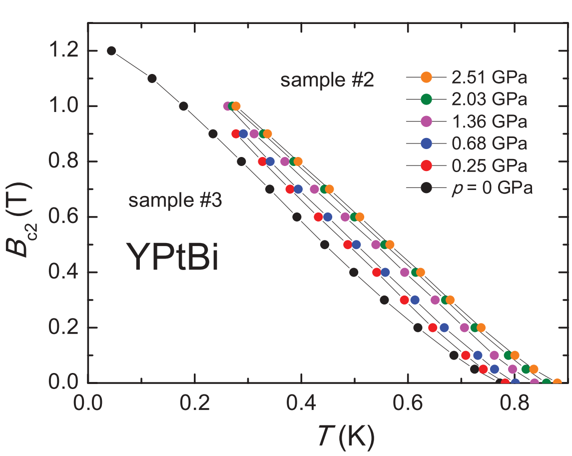

FIG. 4. (Color online) Temperature variation of the upper critical field $B_{c2}(T)$ at pressures of 0, 0.25, 0.68, 1.36, 2.03, and 2.51 GPa (from bottom to top). Data at $p = 0$ are taken on sample #3; data under pressure on sample #2.

IV. ANALYSIS AND DISCUSSION

The relatively weak pressure dependence of $\rho(T)$ and the enhancement of T_c with pressure are unexpected for a low carrier density material. For instance in $Cu_xBi_2Se_3$, which has a comparable metallic behavior and low carrier concentration, the resistance is enhanced and T_c decreases under pressure.[22] In that case the variation $T_c(p)$ can be understood qualitatively in a simple model, where $T_c \sim \Theta_D \exp[-1/N(0)V_0]$, with Θ_D the Debye temperature, $N(0) \sim m^* n^{1/3}$ the density of states (with m^* the effective mass), and V_0 the effective interaction parameter.[27] For $Cu_xBi_2Se_3$, n decreases with pressure, and accordingly T_c decreases.[22] For YPtBi, the weak variation of R with pressure (Fig. 1) suggests n is close to pressure independent. Therefore, the increase $T_c(p)$ indicates the product $N(0)V_0$ has a more involved dependence on pressure.

Next we extract parameters that characterize the superconducting state and investigate whether our samples are sufficiently pure to allow for odd-parity superconductivity.[28] From the relation $B_{c2} = \Phi_0/2\pi\xi^2$, where Φ_0 is the flux quantum, we calculate a superconducting coherence length $\xi = 17$ nm. An estimate for the electron mean free path ℓ can be obtained from the relation $\ell = \hbar k_F/\rho_0 n e^2$, assuming a spherical Fermi surface $S_F = 4\pi k_F^2$ with Fermi wave number $k_F = (3\pi^2 n)^{1/3}$. With $n = 2.2 \times 10^{25}$ m^{-3} and $\rho_0 = 1.6 \times 10^{-6}\Omega$ m (see Fig. 1), we calculate $k_F = 0.9 \times 10^9$ m^{-1} and $\ell = 105$ nm. Thus $\ell > \xi$, which tells us YPtBi is in the clean limit. Similar values for ℓ and ξ were obtained in Ref. 1. A more elaborate analysis can be made by employing the slope of the upper critical field dB_{c2}/dT at T_c:[29] $|dB_{c2}/dT|_{T_c} \simeq 4480\gamma\rho_0 + 1.38 \times 10^{35}\gamma^2 T_c/S_F^2$. Assuming $\gamma \sim n^{1/2}$ we estimate for our sample γ =7.3 J/m^3 K^2 based on the value of 2.3 J/m^3 K^2 (Ref. 24) and by taking into account that for our sample n at low T is 10× higher than reported in Ref. 1. With the experimental values $\rho_0 = 1.6 \times 10^{-6}\Omega$ m, $T_c = 0.77$ K, and $|dB_{c2}/dT|_{T_c} = 1.9$ T/K (see Fig. 4, we neglect the weak curvature close to T_c), we calculate $k_F = 0.4 \times 10^9$ m^{-1}, $\xi = 20$ nm, and $\ell = 582$ nm. This confirms $\ell > \xi$. The weak pressure response of the transport parameters justifies the conclusion that the clean limit behavior is also obeyed under pressure.

For a standard weak-coupling spin-singlet superconductor in the clean limit, the orbital critical field is given by $B_{c2}^{\mathrm{orb}}(0) = 0.72T_c|dB_{c2}/dT|_{T_c}$ (Werthamer-Helfand-Hohenberg [WHH] model[30]). If one considers in addition the suppression of the spin-singlet state by paramagnetic limitation,[31,32] the resulting critical field is reduced to $B_{c2}(0) = B_{c2}^{\mathrm{orb}}(0)/\sqrt{1+\alpha^2}$, with the Maki parameter $\alpha = \sqrt{2}B_{c2}^{\mathrm{orb}}(0)/B^P(0)$ (Refs. 30 and 33) and the Pauli limiting field $B^P(0) = 1.86T_c$. For YPtBi we calculate $B_{c2}^{\mathrm{orb}}(0) = 1.05$ T, $B^P(0) = 1.43$ T, $\alpha = 1.04$, and $B_{c2}(0) = 0.73$ T. The latter value is much lower than the experimental value $B_{c2}(0) = 1.24$ T, and we conclude B_{c2} is dominated by the orbital limiting field.

In Fig. 5 we present the B_{c2} data at different pressures in a reduced plot $b^*(t)$, with $b^* = (B_{c2}/T_c)/|dB_{c2}/dT|_{T_c}$ and $t = T/T_c$ the reduced temperature. All the $B_{c2}(T)$ curves collapse onto a single function $b^*(t)$. In Fig. 5 we have also traced the universal B_{c2} curve for a clean orbital limited spin-singlet superconductor within the WHH model.[30] Clearly, the data

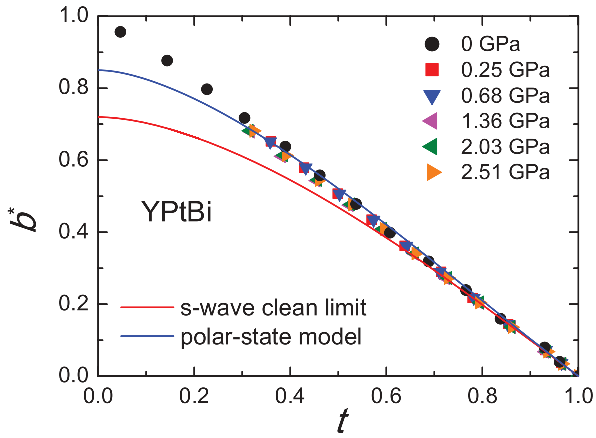

FIG. 5. (Color online) Reduced upper critical field $b^* = [B_{c2}(T)/T_c]/|dB_{c2}/dT|_{T_c}$ as a function of the reduced temperature $t = T/T_c$ at pressures of 0, 0.25, 0.68, 1.36, 2.03, and 2.51 GPa. Notice that we neglected the small tail close to T_c and obtained $|dB_{c2}/dT|_{T_c}$ from the field range $B = 0.1$ to 0.2 T. The red (lower) and blue (upper) full lines represent model calculations for s- and p-wave superconductors, respectively (see text).

deviate from the standard spin-singlet behavior. Notably the fact that our B_{c2} data are well above even these universal values is a strong argument in favor of odd-parity superconductivity. A similar conclusion based on B_{c2} data was drawn for the candidate topological superconductor $Cu_xBi_2Se_3$ (Ref. 22). Finally, we compare the $B_{c2}(T)$ data with the polar-state model function of a spin-triplet superconductor.[34] Overall, the B_{c2} values match the model function better, but significant discrepancies remain. Notably, the unusual quasilinear $b^*(t)$ down to $t/3$ is not accounted for, while below $t/3$ the data exceed the model function values. Clearly, more theoretical work is needed to capture the intricate behavior of mixed spin-singlet and spin-triplet superconductors in an applied magnetic field.

V. SUMMARY

In summary, we have prepared single crystals of the noncentrosymmetric superconductor YPtBi. Superconductivity is confirmed at $T_c = 0.77$ K. Transport measurements demonstrate our crystals exhibit metallic rather than semimetallic behavior. We have investigated the response to pressure of the superconducting phase and find superconductivity is promoted by pressure. The upper-critical field B_{c2} data under pressure collapse onto a single universal curve, which differs from the standard curve of a weak-coupling, orbital-limited, spin-singlet superconductor. The sufficiently large mean free path, the absence of Pauli limiting, and the unusual temperature variation of B_{c2} all point to a dominant odd-parity component in the superconducting order parameter of noncentrosymmetric YPtBi.

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