Strain induced topological non-triviality in YPdBi thin films: A combined experimental plus DFT study

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Abstract:

We report a complementary experimental and theoretical characterization of (110) oriented YPdBi thin-film, grown on MgO (100) substrate, thus engineering a tensile strain \(\sim 3.12\%\) in the YPdBi lattice. The DFT based first principles simulations are used to demonstrate the strain tunable nature (from trivial to inverted) of YPdBi band structure. Calculations of \(Z_2\) invariants confirm the topological non-triviality in the strained lattice. The transport measurements on the film reveal the usual semi-metallic behavior in the temperature range \(3 K \leq T \leq 350 K\). A sharp drop in resistivity is observed at \(\sim 2.2 K\) with critical temperature \(\sim 1.25 K\); however, the resistivity remains finite even down to 0.3 K. This down-turn in resistivity at 2.2 K is found to be magnetic field dependent, finally vanishing at \(B \sim 5 T\). The magneto-transport data show all features of topologically non-trivial surface; \(viz\), a sharp cusp around the low magnetic field region, indicating 2D weak anti-localization \((\alpha \approx 0.50\) and \(L_\phi \propto T^{-0.48}\) and Shubnikov de-Hass (SdH) oscillations at high magnetic fields, in the temperature range \(3 K \leq T \leq 10 K\). A (110) oriented semi-infinite slab of strained YPdBi, simulated to mimic the thin film, shows the presence of electronic pockets with very small effective mass electrons near the Fermi level. Identifying these Fermi pockets as the origin of very mobile electrons on (110) surface, we reach a value of \(E_F \approx 88\) meV; which is in good agreement with the value \((E_F \approx 48\) meV) extracted from the SdH oscillations observed at high magnetic fields in the magneto-resistance data. Our results indicate a possible topological/unconventional superconducting state below 2.2 K and conductance through topological semi-metallic thin film surface above 2.2K. Hence, in this work, we clearly demonstrate the evidences of strain induced topological non-triviality in the YPdBi thin-films.
Introduction

The conventional scheme of classification of materials into metals and insulators have been recently challenged by the discovery of topological insulators which has been under intense current research focus in condensed matter physics. This new state of quantum matter has a fully gapped insulating state in the bulk and topologically protected gapless surface or edge states. Intriguingly, they show low-energy electronic excitations that resemble the Dirac fermions enabling us to explore the physics of these elusive particles in high energy physics using much simpler condensed matter experiments. The half-Heusler alloy family consists of a large collection of semimetals that are predicted to exist in either topologically trivial or non-trivial state. Importantly, the wide variety of Heusler alloys allows precise tuning of the bandgap and band inversion strength by altering their chemical composition. Even more interestingly, recent theoretical studies have indicated the possibility to engineer non-trivial topological states in an otherwise trivial half-Heusler system by strain engineering. An usual approach to demonstrate these non-trivial surface states is by angle resolved photoemission spectroscopy and other surface sensitive techniques. But since the surface states of these materials are topologically protected and conserve time reversal symmetry, an applied external magnetic field can break this symmetry providing a pathway to detect these topologically protected states. This is frequently done by magneto-transport experiments which probe the presence of topologically non-trivial surface states.

The YPdBi (YPB) is a well-established topologically trivial half-Heusler system which was theoretically predicted to undergo a strain-driven transition to a non-trivial state. Single crystal YPB samples have already been established as a topologically non-trivial system based on nuclear magnetic resonance, electron spin resonance and density functional theory (DFT) studies. Although the lattice could be strained by applying uniaxial pressure, an easier way is to grow oriented thin films on carefully selected substrates to induce a lattice strain. A distinct advantage in thin film systems is the large surface/volume ratio making it easier to detect the effect of the surface states on transport properties with a reduced contribution from the bulk. In 2013, Wang reported SdH oscillations and large linear MR in (100) YPB single crystal compound and attributed their results to the high-mobility 3D bulk electron carriers. Recently, an unconventional superconductivity has also been reported in YPB single crystals, which is referred as mixed, singlet-triplet superconductivity.

In this article, we report magneto-transport measurements on (110) oriented strained YPB thin films (~30nm) grown on MgO (100) single crystal substrates to demonstrate the non-trivial nature of the surface states of these oriented YPB films and onset of superconductivity in these strained films below 1 K. We perform DFT based first-principles calculations to show a topologically trivial to non-trivial transition driven by a strained YPB lattice. Furthermore, by constructing a Maximally Localised Wannier Function (MLWF)-based tight-binding model, we calculate the $Z_2$ invariants to show the topologically non-trivial nature of the strained lattice.
Results

Structural characterization

Figure 1a shows the powder XRD pattern and Rietveld refinement of bulk YPB sample. The Rietveld refinement of powder XRD data confirms the \( \text{C1}_b \) crystal structure (\( F\bar{4}3m \) space group) of the sample with lattice constant \( \sim 6.638 \, \text{Å}^{15,24} \). Figure 1b shows the Gonio mode XRD pattern of YPB thin film and the observation of Bragg reflections corresponding to (220) and (440) planes indicate the (110) oriented growth of the film with the expected \( \text{C1}_b \) structure and lattice constant \( \sim 6.845 \, \text{Å} \). This indicates about \( \sim 3.12 \% \) strained lattice of YPB thin films. A very small full width at half maximum (FWHM) of about \( \sim 0.19^\circ \) obtained from the rocking curve (\( \omega-2\theta \)) scan around (220) plane (inset of the Fig. 1b) indicates the high crystallinity and (110) oriented growth of YPB thin film. We estimate the film thickness using specular X-ray reflectivity (XRR) (\( \omega-2\theta \)) scans. Figure 1c shows the experimental and fitted XRR spectra for YPB \( \sim 30 \) nm thin films on a Ta \( \sim 5 \) nm layer with interface roughness \( \sim 1.2 \) nm. Insets of Fig. 1c show the \( \text{C1}_b \) crystal structure of YPB and schematic of Ta (5nm)/ YPB (30nm) bilayer stack. The film topography is analyzed using atomic force microscopy (AFM) and surface roughness \( \sim 1 \) nm is estimated from AFM image as shown in Fig. 1d with the granular growth of the film shown in the tilted 3D AFM image inset.
Figure 1 | Structural characterizations of YPB. (a) Rietveld refinement of YPB powder XRD pattern. (b) Gonio mode XRD pattern of YPB thin film, inset shows rocking curve scan of (220) peak. (c) X-ray reflectivity scan of Ta (5nm)/YPB (30 nm) and corresponding fitting curve in red color. Insets show the $C1_b$ lattice structure of YPB and stacking of Ta/YPB thin films. (d) Topographical AFM image, inset shows corresponding tilted 3D image.

Electrical and Magneto-Transport Characterization

Magnetic field ($H$) – and temperature-dependent resistance ($R$) measurement in a four-point current-biased configuration were performed on unpatterned samples of dimensions 3 mm $\times$ 10 mm. Figure 2a shows the temperature-dependent resistivity ($\rho_{xx}$) data of YPB thin film in the temperature range of 1.9 K – 350 K. The data show a typical semi-metallic behavior in the temperature range 2.2 K $\leq$ T $\leq$ 350 K. Inset of Fig. 1a shows the $R_{xx}$ vs T plot for YPB bulk sample which are in consistent with earlier report on YPB single crystal by Wang. et al. Interestingly, for YPB thin film there is a sharp down-turn in the resistivity below $\sim$ 2.2 K with a corresponding transition width ($\Delta T$) = 0.95 K (T$_C$ $\sim$ 1.25 K), see inset of Fig. 2b. This sharp drop in resistivity could be linked to the onset of superconductivity.

To gain more insight into the possible onset of superconductivity in YPB at low temperatures, we measured this drop in $\rho_{xx}$ in presence of an external magnetic field of increasing strength from 0 T to 9 T applied perpendicular to the film plane. The data, shown in the Fig. 2b, clearly indicates that this resistance drop completely disappears for magnetic fields $\geq$5 T. These measurements were limited by the base temperature of the cryostat at 1.9 K. However, we measured the zero-field resistivity in a separate system with a base temperature of 0.3 K and the data is plotted in the inset of Figure 2a which clearly shows a very sharp drop in resistivity by almost two orders of magnitude from 2.2 K down to 0.3 K. The residual resistivity at the base temperature of the cryostat was 0.05 m$\Omega$-cm.

A series of $R - H$ measurements were performed at various temperatures and the corresponding resistance (called magneto-resistance or MR) change with applied field (perpendicular to film plane) was calculated. Figure 2c shows the MR% of YPB recorded at 1.9 K and 2 K with maximum MR of $\sim$ 35% observed at 1.9 K. The full dependence of MR above this temperature is showed in Figure 2(d) up to a maximum temperature of 50 K. Although large MR is observed for temperatures 1.9 K and 2 K (Figure 2c) where the film shows metallic characteristics, the MR decreases to $\sim$ 2.4% at 3 K and vanishes completely at 50 K as seen in Fig. 2d. We fit our MR results around low magnetic field region (-0.5T to +0.5T) to the well-known HLN model, which describes the conductivity of a two dimensional electron systems with strong spin-orbit interactions under an applied magnetic field. Figures 3a (for $T = 1.9$ K and 2 K) and 3b (3 K $\leq$ T $\leq$ 10 K) show the HLN model fitted longitudinal magneto conductance (\Delta$G_{xx}$ = $G_{xx}(B) - G_{xx}(0)$) data in a strong spin-orbit interaction regime, i.e., when the inelastic scattering time ($\tau_\phi$)$\gg$spin-orbit scattering time ($\tau_{SO}$) and elastic scattering time ($\tau_e$). The HLN equation can be described as follows:

$$\Delta G_{xx} = -\frac{ae^2}{2\pi^2\hbar} \ln \frac{B_\varphi}{B} - \Psi \left(\ln \frac{1 + B_\varphi}{B} \right)$$

(1)
with $B_\varphi = \frac{h}{4eL_\varphi}$, where $h$, $e$ and $L_\varphi$ are the Dirac’s constant, the charge of the electron and the phase coherence length of the carriers, respectively. The function $\Psi$ is the digamma function and the parameter $\alpha$ defines the number of coherent channels, i.e., $\alpha = -0.50$ and $-1$ for single and two coherent channels, respectively. The variation of the HLN fitted parameters $\alpha$ and $L_\varphi$ with temperature ($1.9$ K $\leq T \leq 10$ K) is shown in the Figs. 3c and 3d, respectively. The values of prefactor $\alpha$ and $L_\varphi$ estimated from fitting the $\Delta G_{xx}$ data are $\sim -0.71$ and $162$ nm at $1.9$ K, $\sim -0.82$ and $158$ nm at $2$ K. The WAL parameters $\alpha \sim -1/2$ and $L_\varphi \propto T^{-0.48}$ are extracted in temperature range $3$ K to $10$ K.

To summarize, the data in Fig. 2 shows a typical semi-metallic curve in temperature range $2.2$ K to $350$ K and an onset of superconductivity below $2.2$ K with $T_C \sim 1.25$ K. The sharp drop in resistivity is found to disappear in presence of $H \geq 5$ T. A positive saturating MR $\sim 35\%$ is observed at $1.9$ K and the MR data shows a key signature of topological non-triviality i.e WAL effect around low magnetic fields. Fitting of the WAL to well-known HLN equation indicate the observation of 2D-WAL effect with $\alpha \sim -1/2$, $L_\varphi \propto T^{-0.48}$ above the transition ($T_C \sim 1.25$ K) and contribution of bulk atoms in the conductance below this transition (with $\alpha = -0.71$ at $1.9$ K and $-0.82$ at $2$ K). We will discuss the contribution of surface and bulk atoms to the conductance using DFT in next sections.
Figure 2 | Transport properties of YPB thin film. (a) $\rho_{xx}$ as a function of temperature from 1.9 K to 300 K, inset shows $R_{xx}$ vs T plot for YPB bulk sample. (b) $\rho_{xx}$ vs temperature measured in presence of magnetic field from 0 T to 9 T, inset shows $\rho_{xx}$ measured from 0.3 K to 10 K. (c) MR data at temperatures 1.9 K and 2 K. (d) MR data in the temperature range 3 K ≤ T ≤ 50 K.

Band structure parameters from SdH Oscillations:

In Fig. 4a we have shown the SdH oscillations extracted from the high magnetic field MR data (after the background subtraction) in the temperature range 1.9 K ≤ T ≤ 10 K. The clear SdH oscillations are observed up to 15 K. Above 15K, the oscillatory signal is masked by the background noise. These oscillations are periodic as a function of 1/B and result from the quantization of the Landau levels in high magnetic fields. The inset of the figure shows the fast fourier transformed (FFT) spectra of SdH oscillations, and the extracted single frequency of oscillations is $f_{SdH} \sim 24$ T. The cross sectional area $A_F$ of 2D circular (assumed) Fermi surface normal to the magnetic field can be estimated using the Onsager relation $A_F = \frac{(2\pi e)}{f_{SdH}} \frac{\ell}{h}$. The Fermi wave vector ($k_F$) and sheet carrier concentration ($n_s = k_F^2 / 4\pi$) are estimated as $0.027 \ \text{Å}^{-1}$ and $5.80 \times 10^{11} \ \text{cm}^{-2}$, respectively. The cyclotron effective mass of carriers can be estimated by
Figure 3 | HLN fitting to WAL data. (a) The HLN fit of magneto-conductance $\Delta G_{xx}$ data at 1.9 K and 2 K. (b) HLN fitting in range $3 \leq T \leq 10$ K. (c) Variation of $\alpha$ with temperature. (d) Variation of $L_\phi$ with temperature.

analyzing the damping of oscillations with increase in temperature. The decrease in SdH amplitude with increase in temperature is fitted with the thermal damping term of the standard Lifshitz-Kosevich expression $E_{n}(B) = 2\pi^2 \kappa_{\beta} T / \Delta E_{n}(B) \sinh(2\pi^2 \kappa_{\beta} T / \Delta E_{n}(B))$, and shown in the Fig. 4b. Here, $\kappa_{\beta}$ is Boltzmann’s constant and $\Delta E_{n}(B)$ is the fitting parameter which is related to the cyclotron effective mass ($m^*$) of the carriers as $\Delta E_{n}(B) = \hbar e H / m^*$. The parameter $\Delta E_{n}(B)$ accounts for the splitting of the Landau levels ($n$) in presence of the magnetic field, $B$. The minima and maxima of oscillations in $\Delta R_{xx}$ correspond to the Landau levels $n$ and $n+\frac{1}{2}$, respectively, as shown in the inset of the Fig. 4c. In topologically non-trivial semi-metals, the Berry phase factor $\beta=1/2$ and Berry phase $2\pi\beta=\pi^{1,2}-34$. Berry phase can be estimated from the Landau Level fan diagram, where $n$ data points are plotted as a function of inverse magnetic field and least square fitted to a straight line that result in intercept $\beta$ on $n$ axis (shown in the Fig. 4c). The $\beta=0.46\pm0.1$ and Berry phase $= 0.92\pm0.1$ are estimated from $n$ axis intercept of linear fitting to $(\Delta R_{xx})_{max}$ and $(\Delta R_{xx})_{min}$ data points. The Fermi velocity of carriers ($V_F = \hbar k_F / m^*$) and position of Fermi level from linear bands crossing ($E_F = m^* V_F^2$) are estimated as $\sim 2.70 \times 10^5$ ms$^{-1}$ and 48 meV, respectively. The transport lifetime and mean free path of the carriers can be estimated using dingle plot of SdH oscillations observed at any temperature $T$ by extracting the slope of $\ln(\Delta R_{xx}(B)/\Delta R_{xx}(0))B \sinh(2\pi \kappa_{\beta} T / \Delta E_{n}(B))$ vs $1/B$ plot. Figure 4d shows the dingle plots at 1.9 K, 3 K and 4 K, the slope of linear fitting to the data points gives dingle temperature $T_D \sim 5$ K. The transport lifetime ($\tau$) and mean free path ($l$) of carriers are estimated using the relations, $\tau = \hbar / (2\pi T_D)$ and $l = V_F \tau$ as $2.43 \times 10^{-13}$ s and 66 nm, respectively. The $m^*$ and the carrier mobility ($\mu_s = e\tau /m^*$) are obtained as $\sim 0.12$ m$\_c$ and 3694 cm$^2$V$^{-1}$s$^{-1}$, respectively. The parameters extracted from different fits are listed in the Table 1.

Table 1 | Different parameters extracted from the fit of SdH data

| $f_{SdH}$ (T) | $n_s$ ($10^{11}$ cm$^{-2}$) | $m^*$ ($m_e$) | $k_F$ (Å$^{-1}$) | $V_F$ ($10^5$ ms$^{-1}$) | $E_F$ (meV) | $\tau$ ($10^{-13}$ s) | $l$ (nm) | $\mu_s$ (cm$^2$V$^{-1}$s$^{-1}$) |
|----------------|-----------------|---------|-------------|-----------------|------|-------|------|-----------------|
| 24 | 5.80 | 0.12 | 0.027 | 2.70 | $\sim 48$ | 2.43 | $\sim 66$ | $\sim 3694$ |
Figure 4 | Analysis of SdH data. (a) The SdH oscillations at temperatures in the range from 1.9 K and 10 K. Inset shows the corresponding FFT spectra. (b) Standard L-K fit of temperature dependent SdH amplitudes. (c) The Landau level fan diagram of SdH maxima and minima. Inset shows the Landau level assignment to SdH data at 1.9K. (d) Dingle plot of YPB at 1.9 K, 3 K and 4 K.

Electronic structure of YPB bulk and (110) oriented YPB thin film:

The experimental results reported so far strongly suggest topologically non-trivial band structure of strained YPB thin films. In order to confirm this topologically non-trivial nature, we perform DFT-based first principles calculations. The crystal structure of YPB is rhombohedral associated with the space group F̅3m. The unit cell contains three atoms where atoms Y, Pd and Bi occupy the (0.5,0.5,0.5), (0.25,0.25,0.25) and (0.0,0.0,0.0) Wyckoff positions, respectively. We begin by calculating the equilibrium lattice constant, which is obtained by minimizing total energy with respect to the lattice parameter. The calculated lattice constant of 6.570 Å agrees well with the measured value, 6.638 Å. The difference between the two results can be attributed to the use of LDA pseudopotentials in this study.

In Fig. 5a we have shown the electronic band structure of unstrained and strained YPB bulk. The band dispersion of unstrained YPB lattice shows a doubly degenerate Γ₆ lying above the quadruply degenerate Γ₈ indicating a topologically trivial band structure, in agreement with the previously reported theoretical and experimental studies on YPB. The band structure of the strained YPB lattice is calculated with the lattice constant of 6.774 Å which corresponds to
3.12% tensile strain, as estimated from the XRD results of (110) oriented YPB thin films. The band dispersion of strained YPB clearly shows a band inversion, which suggests topological non-triviality in the strained lattice of YPB. Calculated value of strong $Z_2$ index $v_0=1$, confirms the topologically non-trivial nature of the strained bulk. Our DFT results show a strong topological nature for a strained YPB lattice which closely agrees with our experimental results. Moreover, the conduction and valence bands of strained YPB touch at $\Gamma$ point and obey a quadratic dispersion relation. We calculate the curvature of the valence bands near the $\Gamma$ point and estimate the inertial effective mass ($m^{**}$) of electron at the center of the Brillouin zone. The value of $m^{**}=0.048 m_e$ is indicative of the origin of high mobility electrons at $\Gamma$ point in the case of strained bulk YPB.

Next, we investigate the electronic structure of strained (110) oriented YPB thin film. To simulate the film, we create a semi-infinite slab made of 20 atomic layers with strained lattice constant of 6.774 Å, as shown in the Fig. 5b. A vacuum of approximately 20 Å is placed at the end of the slab to simulate the semi-infinite boundary condition of the film. Out of the 20 atomic layers of the slab, two outer layers each from top and bottom are referred as the surface layers and the rest 16 layers are referred as bulk layers. To assess the contribution of the surface states to electronic transport through the film, we calculate the $k$-resolved density of states of the slab as shown in figure 5c. Electronic density from the surface layers are shown in red and that from the bulk layers is shown in cyan color. It is interesting to observe the two bands which create Fermi pockets near the $\Gamma$ point have contribution from both surface atoms as well as bulk of the slab.

Interestingly, as in the case of strained bulk lattice, a parabolic band dispersion is seen at the $\Gamma$ point (Fig. 5c). Two bands cross the Fermi energy near $\Gamma$ point, creating the Fermi pockets. In order to precisely calculate the inertial effective mass $m^{**}$ of the electrons originating from this Fermi pocket, we separated out these two bands (see Fig. 5d) and calculated the curvature at the local maxima ($\Gamma$ point) of these bands. The calculated $m^{**}$ tensor for these two bands at $\Gamma$ point are

$$
(m^{**})_{\text{band}1} = \begin{pmatrix}
-0.0028 & 0.0000 \\
0.0000 & -0.0368
\end{pmatrix} \quad \text{and} \quad (2)
$$

$$
(m^{**})_{\text{band}2} = \begin{pmatrix}
-0.0327 & 0.0000 \\
0.0000 & -0.0416
\end{pmatrix} \quad \text{(3)}
$$

normalized with respect to the rest mass of the electron, $m_e$. Such low values of $m^{**}$ give rise to the high mobility of electrons and SdH oscillations in (110) oriented YPB thin film. Identifying these Fermi pockets as the origin of very mobile electrons on (110) surface, we reach a value of $E^S_\Gamma=88$ meV, which is of the same order of magnitude with experimentally observed value of $E^S_\Gamma$, as given in Table 1. It is noteworthy that, since the dispersion shown around $\Gamma$ in Fig. 5c is approximately parabolic, effective mass calculated through curvature is reasonably accurate. However, the scatterings at defects and impurities are expected to affect the experimentally obtained mobility and effective mass of the electrons originated from the electronic pockets. That is why, the $m^{**}$ obtained theoretically is much lower than the experimentally measured value of effective mass from Table 1.
Figure 5 | Band structure of bulk YPB and strained thin films. (a) Electronic band structure calculated with equilibrium lattice constant 6.570 Å and strained lattice constant 6.774 Å. (b) Lattice structure of semi-infinite (110) oriented slab of YPB with vacuum on both sides. (c) The K-resolved density of states showing contribution from surface atoms. Red color represents the contribution of atoms from the surface layers and cyan color represents the contribution from bulk layers. (d) E-k dispersion of two bands crossing the Fermi energy.

Discussion:

The magneto-transport measurements indicate the topological nontrivial nature of (110) oriented YPB thin films at low temperatures. A sharp drop in $\rho_{xx}$ curve is observed at $\sim 2.2$ K with $T_C \sim 1.25$ K and this drop disappear in presence of magnetic field $\geq 5$ T. Similar sharp drop in
temperature dependent resistance in temperature range 2 K to 0.5 K (T_c ~ 1.3 K and 1.2 K with \( \Delta T = 0.26 \) K) had been reported by Radmanesh et al. in YPB single crystals\(^{22}\). This was addressed as an unconventional superconductivity in YPB single crystals. It should be noted that in earlier works on YPtBi non-trivial topological semi-metal, having similar band structure to non-trivial strained YPB\(^{8,9}\), many groups have reported unconventional/topological superconductivity at very low temperatures\(^{36-38}\). This unconventional superconducting state is attributed to spin-3/2 quasi-particle electronic structure of YPtBi topological semi-metal by Kim et al.\(^{39}\). The \( \rho_{xx} \) behavior observed in our strained YPB thin film resembles the unconventional superconductivity observed by Pavlosiuk et al. in YPtBi single crystal (T_c~0.97 K and \( \Delta T = 0.45 \) K)\(^{37}\).

A sharp rise in MR around low magnetic field is observed. In topologically non-trivial materials, such a sharp rise in resistances in the low-field region, arise from the destructive interference of spin 1/2 carrier wave functions having \( \pi \) Berry phase associated with them and is referred to as the WAL effect\(^{39}\). The HLN fitting to WAL data at 1.9 K and 2 K results in fitting parameter \( \alpha \sim -0.82 \) and ~-0.71, respectively. The metallic like \( \rho_{xx} \) behavior and \( \alpha \) in the range -1 < \( \alpha \) < -0.5 at 1.9 K and 2 K indicate at-least a partial contribution from bulk electrons to the surface channel conductance. The WAL parameters \( \alpha \sim -0.51 \) and \( L_\varphi \sim T^{-0.48} \) are extracted in temperature range 3 K to 10 K. This validates the topological non-triviality of strained YPB lattice and observation of 2D WAL above 3K in thin film. The observation of metallic like \( \rho_{xx} \) behavior with \( \Delta T = 0.95 \) K and \( \alpha = -0.82 \) and -0.71 at 1.9 K and 2 K respectively, indicate partial coupling of surface and bulk channels. As discernible from the Fig. 3d, \( L_\varphi \) decreases with increase in temperature and follows \( L_\varphi \propto T^{-0.48} \) power law dependence in the temperature range 3 K ≤ \( T \leq 10 \) K. This, along with the \( \alpha = -0.50 \), indicate the observation of 2D WAL effect\(^{28,40}\) and topological non-triviality\(^{37}\) in temperature range 3 K ≤ \( T \leq 10 \) K. The \( L_\varphi \) observed at 1.9 K (166 nm) is ~ 3 times the \( L_\varphi \) at 3K (60 nm), which can be due to the onset of topological superconducting state below 2.2K. Hence, the power law fit to \( L_\varphi \) at 1.9 K and 2 K shows deviation in the fitted curve (see Fig. 3(d)). The SdH oscillations are also observed in high field MR data which are another signature of topological non-triviality. The electronic band structure parameters are estimated from L-K fitting of SdH data and \( m^* \) of carriers \( \sim 0.12 m_e \) with \( \mu_e \sim 3694 \text{ cm}^2\text{V}^{-1}\text{s}^{-1} \) is extracted. These values are very similar to those reported by Butch et al. (0.15 \( m_e \), 3500 \( \text{cm}^2\text{V}^{-1}\text{s}^{-1} \)) and better than those reported by Pavlosiuk et al. (0.22 \( m_e \), 1486 \( \text{cm}^2\text{V}^{-1}\text{s}^{-1} \)) for YPtBi single crystals below 10K\(^{37,38}\).

The complementary first-principles based DFT calculations indicate the fact that although the bulk YPB is topologically trivial, the strained (3.118%) YPB thin film is topologically non-trivial. This confirms the strain tunability of YPB band structure from positive to negative band inversion as predicted by Chadov et al.\(^9\). The DFT simulations of semi-infinite slab of (110) oriented strained YPB show the existence of Fermi pockets contributed mostly by bulk bands. We attribute the observation of SdH oscillations and very small \( m^* \) with high \( \mu_e \) (~3694 cm\(^2\text{V}^{-1}\text{s}^{-1} \)) to these electrons from the Fermi pockets. The fact that we observe superconductivity in a topologically non-trivial system is quite interesting and it hints at unconventional order parameter symmetries. These findings indicate the observation of a topological non-trivial state in strained YPB and possible topological superconductivity below 2.2 K with conductance through topologically non-trivial surface above 2.2K. Conclusively this paper demonstrates non-trivial topological nature of strained YPdBi which has long been predicted to undergo a trivial to non-trivial transition with strain.
Methods:

Sample preparation: The YPB thin films are grown using pulsed laser deposition system with KrF excimer pulsed laser source (λ = 248 nm). The energy density of source is about ~ 1.1 J/cm² and chamber base pressure ~ 3 × 10⁻⁷ mbar. Laser pulses are bombarded on 1” YPB target, prepared using RF induction melting method²⁶. Thin films are grown on MgO (100) substrate with ~ 5 nm Ta seed layer at 270 °C insitu substrate temperatures.

Experimental characterization: The crystal structure and film thickness are determined using Cu Kα Panalytical X’pert highscore Diffractogram by using X-ray diffraction and x-ray reflectivity techniques. The surface topography is studied using Bruker Dimension 3100 atomic force microscope (AFM). The electrical contacts for transport measurements are prepared using copper wires and cured with silver paste. The magneto-transport properties of thin films with dimensions 3 × 10 mm are studied using Quantum Design 9T PPMS system in the temperature range from 1.9 K to 300 K. The mK transport studies are carried out using Cryogen Free Measurement System from Cryogenic Limited.

First-principles simulations: Density functional theory based first-principles calculations using the projector augmented wave (PAW)¹¹,⁴² method as implemented in Vienna ab-initio simulation package (VASP)¹³–⁴⁶ are used in this paper. In order to incorporate the exchange-correlation from electrons, we use the local density approximation (LDA), as formulated by Ceperley and Adler⁴⁷ in all the calculations. The semicore electrons 3s and 3p for Y and 5d for Bi are treated as the valence electrons. The convergence criterion for self-consistent field calculation of energy and band structure calculations was chosen as 10⁻⁸ eV, and the residual forces for relaxation calculations were minimized down to 5×10⁻⁵ eV/Å per atom. The energy cutoff of plane wave basis was chosen as 400 eV for all calculations. A Monkhorst-Pack⁴⁷ k-mesh of 13×13×13 and 13×13×1 are used for bulk and slab calculations, respectively. A maximally-localized Wannier function (MLWF) based tight binding model as implemented in Wannier90⁴⁸,⁴⁹ is used to calculate the Z² invariants of strained YPB. To account for relativistic correction, we included spin-orbit coupling in all the simulations.

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Contributions:
V.B. performed the experimental work and has done the complete analysis of results. A.B. performed the theoretical simulations that supported the understanding of the results. S.S. performed mK resistivity measurement with the help of N.B. DFT calculations performed by A.B. are supervised by B.K.M. V.V.K and N.B helped in formation of the manuscript with their critical comments. R.C. conceived the idea and supervised the work.

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