A pressure-induced topological phase with large Berry curvature in Pb$_{1-x}$Sn$_x$Te

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The picture of how a gap closes in a semiconductor has been radically transformed by topological concepts. Instead of the gap closing and immediately reopening, topological arguments predict that, in the absence of inversion symmetry, a metallic phase protected by Weyl nodes persists over a finite interval of the tuning parameter (for example, pressure $P$). The gap reappears when the Weyl nodes mutually annihilate. We report evidence that Pb$_{1-x}$Sn$_x$Te exhibits this topological metallic phase. Using pressure to tune the gap, we have tracked the nucleation of a Fermi surface droplet that rapidly grows in volume with $P$. In the metallic state, we observe a large Berry curvature, which dominates the Hall effect. Moreover, a giant negative magnetoresistance is observed in the insulating side of phase boundaries, in accord with ab initio calculations. The results confirm the existence of a topological metallic phase over a finite pressure interval.

INTRODUCTION

Topological concepts have greatly clarified the role of symmetry in protecting electronic states in a host of materials. In bulk semiconductors, topological insights have revised the picture of how the energy gap closes (say, under pressure $P$). In the old picture, the gap closes at an “accidental” value of $P$ before reopening at higher $P$. The new view (1–4) predicts instead that, when inversion symmetry is broken, a gapless metallic state featuring pairs of Weyl nodes persists over a field interval ($P_1$ to $P_2$). They act as sources and sinks of Berry curvature (an effective magnetic field in $k$ space). The metallic phase is protected because the nodes come in pairs with opposite chiralities ($\chi = \pm 1$). Hence, they cannot be removed except by mutual annihilation (which eventually occurs at the higher pressure $P_2$). To date, these predictions have not been tested.

Here, we show that Pb$_{1-x}$Sn$_x$Te exhibits a pressure-induced metallic phase described by the Weyl scenario. The Pb-based rock salts (5–7) have been identified as topological crystalline insulators with surface states protected by mirror symmetry (8–12). We focus on their Dirac-like bulk states (13, 14), which occur at the $L$ points of the Brillouin zone (BZ) surface. Pb$_{1-x}$Sn$_x$Te exhibits an insulator-to-metal (IM) transition at $P \approx 10$ kbar (7). However, the IM transition is little explored. We report that the metallic state appears by nucleating 12 small Fermi surface (FS) nodes. The breaking of time-reversal symmetry (TRS) in applied $B$ leads to a large Berry curvature $\Omega$. Finally, we also observe an anomalously large negative magnetoresistance (MR), which is anticipated in the Weyl scenario.

RESULTS

Phase diagram under pressure

Crystals of Pb$_{1-x}$Sn$_x$Te were grown by the vertical Bridgman technique (see Materials and Methods). Transport measurements at temperatures $T$ down to 2 K were carried out in a Be-Cu pressure cell (with a maximum pressure of $P_{\text{max}} \approx 28$ kbar) on four samples with Sn contents $x = 0.5$ (samples A1 and A2), 0.32 (Q1), and 0.25 (E1) (Table 1). In A1 and A2, indium (6%) was added to tune the chemical potential (see Materials and Methods).

Figure 1 provides an overview of the IM transitions in samples A2 and E1. As $P$ increases from 0 kbar (ambient pressure) to 25.4 kbar, the resistivity profile $\rho$ versus $T$ changes from insulating to metallic behavior in A2 (Fig. 1A). Close examination reveals a kink in $\rho$, indicating a sharp transition at $T_c = 62 \pm 10$ K (arrows in inset). Figure 1B shows the large negative magnetoresistance (MR), which is anticipated in the two insulating phases.

The end member SnTe is known to be ferroelectric (FE) (15), but the existence of FE distortion is less obvious for finite Pb content. To establish inversion symmetry breaking, we performed dielectric measurements (see Materials and Methods) on sample E1, which has a very large $\rho$ below 10 K ($>10^4 \Omega$ cm). By varying the $E$-field (12→100 V/cm), we show that a large spontaneous dielectric response $\epsilon_s \sim 5 \times 10^4$ exists in the limit $E \rightarrow 0$ (Fig. 1C, inset). The spontaneous polarization $P_s$ provides direct evidence that the insulating state below $P_1$ in E1 is FE. Although dielectric measurements cannot be performed in A2 (carrier screening is too strong), the kink in $\rho$ (arrow) implies that $P_s$ appears at 62 to 70 K.

In parallel, we performed ab initio calculations (see details in the Supplementary Materials), in which the lattice parameter $a$ is varied to simulate pressure. To break inversion symmetry, we assumed a weak FE displacement $d || [111]$. The calculations reveal that, above $P_1$, two pairs of Weyl nodes appear near each of the points $L_1, L_2$, and $L_3$ (these are equivalent in zero $B$; see Fig. 1, E and F). As $P$ increases, the 12 nodes trace out elliptical orbits (shown expanded by a factor of 10 relative to the BZ caliper) and eventually annihilate pairwise (indicated by black dots), consistent with the scenario described by Murakami (2) and Murakami and Kuga (3). The red and blue arcs refer to nodes with
$\chi = 1$ and $-1$, respectively. The splitting of the node at $L_0$ occurs in a much narrower pressure interval.

**Quantum oscillations**

The samples' high mobilities $\mu$ (20,000 to $4 \times 10^6$ cm$^2$/V·s; see Table 1) allow us to “count” the number of FS pockets by monitoring the Shubnikov–de Haas (SdH) oscillations. As shown in Fig. 1 (B and D), $\sigma$ increases steeply with the reduced pressure $\Delta P = P - P_1$. Figure 2A shows the resistivity $\rho_{xx}$ measured in sample A2 in a transverse magnetic field $B$ ($||z$) at selected values of $P$. From the linear variation of $1/B_n$ versus the integers $n$ (where $B_n$ is the peak field in $\rho_{xx}$; see Fig. 2B), we find that the FS caliper area $S_F$ increases from 1.6 to 2.7 T between 19 and 25.4 kbar. The most prominent peak in Fig. 2A corresponds to the $n = 1$ Landau level (LL). The SdH-derived Fermi wave vector $k_F$ corresponds to a hole density $n_{SDH} = \frac{3}{2} \pi k_F^3 / (2\pi)^3$ per spin (assuming a spherical FS).

The sharp increase in hole density is also evident in the Hall resistivity $\rho_{yx}$ (which is $B$-linear in weak $B$). To highlight its behavior, we plot the ratio $\rho_{yx}/n_e B$ versus $B$ (Fig. 2C). In weak $B$ (for example, $|B| < 3.5$ T in the top curve), the ratio is $B$-independent, which allows the ratio to be identified with the Hall density $n_H$ (the abrupt increase above 3 T arises from the interesting anomalous Hall term discussed below). From $n_{H}$, we derive $\mu \sim 1.8 \times 10^4$ and $2.86 \times 10^4$ cm$^2$/V·s in A1 and A2, respectively.

Crucially, we find that $n_H$ always exceeds $n_{SDH}$ by an order of magnitude. This implies a large number $N_F$ of identical pockets. The ratio $n_{H}/n_{SDH} = N_F$ equals $12 \pm 1$ over the whole pressure interval (Fig. 2B, inset). Because a smaller $N_F$ (for example, 4, 6, or 8) can be excluded, the results strongly support the choice $d || [111]$, which leads to three equivalent $L$ points.

**Anomalous Hall effect**

We next describe the evidence for a topological metallic phase. The Hall resistivity $\rho_{yx}$ displays a highly unusual field profile. As $B$

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**Table 1. Parameters of samples of Pb$_{1-x}$Sn$_x$Te investigated.** Columns 2, 3, 4, and 5 report the Sn content $x$, the mobility $\mu$, the Hall carrier density $n_H$, and the conductivity $\sigma$ (at $B = 0$), respectively. The minus sign in $n_H$ (sample Q1) indicates $n$-type carriers. All quantities in the table were measured at 5 K at the pressure $P$ given in the last column. Samples A1 and A2 are slightly doped with In to tune the chemical potential [composition (Pb$_{0.5}$Sn$_{0.5}$)$_1$, (In)$_{0.1}$Te$_{0.9}$].

| Sample | $x$ | $\mu$ (cm$^2$/V·s) | $n_H$ (cm$^{-3}$) | $\sigma$ (mΩ·cm$^{-1}$) | $P$ (kbar) |
|--------|----|--------------------|------------------|-----------------|-------------|
| A1     | 0.5 | 18,000             | 1.59 $\times 10^{27}$ | 0.41            | 25          |
| A2     | 0.5 | 29,000             | 1.56 $\times 10^{27}$ | 0.68            | 25.4        |
| E1     | 0.25| 500,000            | 9.35 $\times 10^{15}$ | 0.70            | 21.7        |
| Q1     | 0.32| 4.2 $\times 10^6$  | -1.05 $\times 10^{16}$ | 7.02            | 21          |

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**Fig. 1.** The phase diagram of Pb$_{1-x}$Sn$_x$Te inferred from the resistivity $\rho$ versus temperature $T$ and pressure $P$. (A) Curves of $\rho$ versus $T$ in sample A2 ($x = 0.5$) in zero $B$ measured at selected $P$. At 5 K, $\rho$ decreases by four orders of magnitude at $P\sim 25$ kbar (the IM transition). The inset shows the kinks (arrows) in $\rho$ between 62 and 70 K, which signal a transition to a state with broken inversion symmetry. (B) Steep increase of conductivity $\sigma = 1/\rho$ at 5 K in the metallic phase (shaded in blue; $P > P_1$). (C) $\rho$ versus $T$ at selected $P$ in sample E1 ($x = 0.25$). The insulating state is recovered at $P_2 \sim 25$ kbar. The inset plots the dielectric response $\varepsilon_1$, measured versus applied electric field $E$ at 2 K and ambient $P$ (a spontaneous value $\varepsilon_1 \sim 5 \times 10^4$ is measured as $E \rightarrow 0$). (D) $\sigma$ versus $P$ at 5 K to display the metallic state in E1 (shaded in blue) sandwiched between $P_1$ and $P_2$. (E and F) Calculated Weyl node trajectories (Supplementary Materials), magnified 10x relative to the BZ scale (with $B = 0$). In (E), the vector $\mathbf{d} || [111]$ (arrow) is the assumed FE displacement. (F) Top view (sighting $||d$). Under pressure, the 12 Weyl nodes at $L_0$, $L_1$, and $L_2$ trace out elliptical orbits until they annihilate at the black points. The Weyl nodes at $L_0$ trace an orbit that undulates about a circular path (over a restricted pressure interval (Supplementary Materials)).
increases, the initial B-linear behavior abruptly changes, bending over to a nominally flat profile (Fig. 3A). At first glance, this recalls the anomalous Hall effect (AHE) in a ferromagnet (16) where the intrinsic AHE arises from a large Berry curvature rendered finite by the spontaneous breaking of TRS, but there is a subtle difference. In PbSnTe, TRS remains unbroken under P, so the AHE should be absent in the Weyl phase if B = 0 (Ω cancels pairwise between Weyl nodes with χ = ±1). However, when TRS is broken in field B, the cancellation is spoiled by the Zeeman energy (see below). The field Ω leads to a large AHE signal. We remark that, in weak B (with Ω negligible), the initial slope of ρyx is dominated by the ordinary Hall effect, as evidenced by the linearity of nH versus ρSdH in Fig. 2B [by contrast, in a ferromagnet, the AHE term is dominant even in weak B, so the weak-B ρyx and nH are unrelated (16)].

The total (observed) Hall conductivity σyx is the sum of the conventional Hall and anomalous Hall conductivities, σyx and σyx AHE, respectively (Fig. 3B). With σyx given by the Druede expression, we find that a good fit to σyx is achieved if we assume σyx AHE = σyx AHE g(x), where σyx AHE is the AHE amplitude and g(x) is the smoothed step function 1/(e + x) + 1, with x being a reduced field (Supplementary Materials). In terms of Ω, σyx AHE is given by (16)

$$\sigma_{yx}^{AHE} = \frac{e}{(2\pi)^2} \int d^3k \text{det}_k \left( e \Omega_{L} / n_{tot} \right)$$

where f_k is the Fermi-Dirac distribution, Ω_L is the Berry curvature averaged over the FS, and n_{tot} is the total carrier density. From the fits at each P, we can track the variation of ⟨Ω_L⟩ ~ σyx AHE / n_{tot} versus P. As shown in Fig. 3C, the curvature ⟨Ω_L⟩ is negligible below P_1 but becomes large in the metallic phase, consistent with the Weyl scenario.

In Fig. 3B, we plot the observed σyx (solid curves) together with the Drude curve for σyx N (dashed curves). Their difference is σyx AHE (shaded region in the curve at 25 kbar). Similar results are obtained in A2 and E1 (Supplementary Materials). σyx grows quite abruptly at an onset field B_A close to where the system enters the lowest (n = 0) LL. Above B_A, the increasing dominance of the AHE current accounts for the abrupt bending of σyx already noted in Fig. 3A, as well as the sharp increase above B_A in ρSdH/Be in Fig. 2C. The observation that σyx AHE is most prominent within the n = 0 LL (which is strictly chiral for Weyl fermions) suggests to us that it is intimately related to the chirality of the nodes.

Each Weyl node acts as a source (χ = 1) or sink (χ = −1) of Ω. As mentioned, in zero B, TRS requires the net sum of Ω over each pair of Weyl nodes to vanish (Fig. 3D). The ab initio calculations (Supplementary Materials) reveal how this cancellation is spoiled when TRS is broken in finite field B. A finite Zeeman field λ shifts the band energies, depending on their spin texture. This increases the k-space separation and Fermi energy of one pair of nodes, say w_1^↑, while reducing them in the other w_2^↑ (Fig. 3D). The unbalancing creates a finite Ω (hence, σyx AHE) that grows with B (Supplementary Materials).

**Giant MR**

Perhaps the most marked feature in Pb_{1-x}Sn_xTe is the appearance of giant negative MR at pressures just above P_2. In Fig. 4A, we show the
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MR curves in sample Q1 for selected T with P fixed at 28 kbar (roughly 3 kbar above P2). At 4.3 K, ρxx decreases by a factor of 30 as B increases to 10 T (aside from a slight dip feature below 0.5 T). In Fig. 4B, similar curves for E1 (at pressure B = 25.4 kbar) show an even larger negative MR (the weak-B dip feature is more prominent as well). The large negative MR is steadily suppressed as we increase P beyond the P2 boundary. The negative MR magnitude is similar in magnitude in both the transverse MR and longitudinal MR geometries (B || z and B || x, respectively). This implies a Zeeman spin mechanism. Finally, we note that, in both Q1 and E1, ρxx measured at 10 T decreases as T → 5 K (that is, the system is metallic).

**DISCUSSION**

The anomalously large changes in ρxx imply that the insulating state (at zero B) is converted to a metallic state in finite B. This is confirmed in the ab initio calculation (Supplementary Materials). A large λ favors the Weyl phase (the left V-shaped yellow region in Fig. 4C). As the phase boundary now tilts into the insulating side, the metallic phase is reen-trant in increasing B. The observation of the giant negative MR provides further evidence in support of the Weyl node scenario.

As predicted in previous studies (1–4), gap closing in materials lacking inversion symmetry leads to a metallic phase that is protected by the distinct chirality of Weyl nodes. Pb1−xSnTe is an instructive first example. Increasing pressure P drives an IM transition at P1, with ρ (at 5 K) falling by four to seven orders of magnitude. Above P1, the growth of the FS calipers is tracked by large SdH oscillations. The number of nodes (12) is consistent with the appearance of four Weyl nodes at each of the 3 L1 points on the BZ surface. The Berry curvature, rendered finite in B, leads to an AHE that is most prominent in the n = 0 LL. Finally, we find that the boundary P2 is shifted in finite B. The reen-trance of the metallic phase leads to a marked decrease in ρxx by a factor of 30 to 50.

**MATERIALS AND METHODS**

**Crystal growth**

Single crystals of Pb1−xSnTe were grown by the conventional vertical Bridgman technique. High-purity elements (5N) with the targeted values of x were sealed in carbon-coated quartz tubes under a high vacuum of ~10−5 mbar. The ampoules were heated at 1050°C for 12 hours. To ensure homogeneous mixing of the melt and to avoid bubble formation in the bottom, we stirred the ampoules. The ampoules were slowly lowered through the crystallization zone of the furnace, at the rate of 1 mm/hour. High-quality single-crystal boules of length ~10 cm were obtained. The crystal boules were cut into segments of 1 cm to investigate the bulk electronic properties along the boule length. The crystals were easily cleavable along different crystallographic planes.

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Fig. 4. Large, negative MR. A large isotropic MR is observed when \( P \) is fixed just above \( P_g \) in samples Q1 and E1. (A) \( \rho_{xx} \) versus \( B \) in Q1 (\( x = 0.32 \)) at selected \( T \), with \( P = 28 \text{ kbar} \). At \( P > P_g \), both samples are insulators at \( B = 0 \text{ T} \). However, at \( B = 10 \text{ T} \), both are metallic (\( \rho_{xx} \) decreases with \( T \)). In (B), similar curves show an even larger negative MR in sample E1 (\( x = 0.25 \)). (C) Ab initio phase diagram (Supplementary Materials) in the plane of \( a \) versus \( \lambda \) at \( L_1 \) for \( B \parallel [\bar{1} \bar{1} \bar{2}] \). With increasing \( \lambda \), the Weyl node annihilation boundary (left V-shaped wedge shaded yellow) expands. A weaker expansion occurs at the creation boundary. (D) Effect of \( B \) (yellow arrow) on the locations of the Weyl nodes around \( L_1 \), \( L_2 \), and \( L_3 \).

A major difficulty in the rock salts is having to ensure that the chemical potential of the alloy lies within the bulk gap (otherwise, the pressure-induced changes to the gap will not be observable). To achieve this goal in crystals with Sn content \( x = 0.5 \), we have found it expedient to dope the starting material with indium [at the 6% level, with composition (\( \text{Pb}_{0.5} \text{Sn}_{0.5} \))\text{In}\text{Te}, with \( y = 0.06 \)]. Indium doping has previously been carried out and investigated by several groups to understand the superconducting phase in \( \text{Pb}_{1-x} \text{Sn}_x \text{Te} (17–19) \). Zhong et al. (19) have reported that In-doped \( \text{Pb}_{1-x} \text{Sn}_x \text{Te} (x = 0.5) \) induces an insulating behavior. However, in our judgment, the precise role of In doping in the Pb-based rock salts is not well understood and merits further detailed investigation.

The x-ray diffractograms recorded for two powdered specimens of two typical samples are shown in fig. S4. The grown crystals were single-phased. The diffraction peaks were in very close agreement with the rock salt crystal structure of space group \( \text{Fm} \bar{3} m \).

Some of the parameters measured in the four samples investigated (A1, A2, E1, and Q1) are reported in Table 1. The mobilities in E1 (p-type) and Q1 (n-type) were very high (500,000 and 4.2 \( \times 10^6 \) cm\(^2\)/V\(s\), respectively). Although the samples with \( x = 0.50 \) (A1 and A2) had lower mobilities (18,000 and 29,000 cm\(^2\)/V\(s\), respectively), clear SdH oscillations were observed above \( P_g \).

**Measurement of dielectric constant**

We provide more details on the measurements of the relative dielectric constants \( \varepsilon_r \). We adopted the (modified) Sawyer-Tower method (20, 21).

The circuit of the original Sawyer-Tower method is shown in Fig. 5A. Figure 5B shows the modified method using an operational amplifier (op-amp) (21).

For the setup shown in Fig. 5A, the sample with a capacitance component \( C_0 \) and a resistance component \( R_0 \) was connected in a series with a known reference capacitance \( C_0 \gg C_r \). The reference capacitance \( C_0 \) was connected in parallel with a fixed resistor \( R_0 \) in series with an adjustable voltage source \( V_0 \) (or, equivalently, a variable resistor \( R_0 \)) that was set such that the voltage \( V_0 \) is in phase with voltage \( V_x \), where \( V_x \) and \( V_y \) represent the voltages across the whole electrical circuit and the reference capacitor \( C_0 \), respectively. Because \( C_0 \gg C_r \) was satisfied, the following relations hold: \( V_x \sim V_y \sim V_0 / C_0 \ll V_x \). Here, \( V_x \) is the voltage applied across the sample. This means that point M in the figure can be treated as a virtual ground. This yields the condition \( V_0/R_0 \sim V_y/R_x \).

The setup in Fig. 5B is the same as that in Fig. 5A except that the op-amp is used to provide a more stable virtual ground at point M. From point M, current \( I_y \) was driven to the op-amp connected to \( C_2 \) and \( R_2 \) in parallel. Here, a large resistor \( R_3 (R_3C_2 \gg 1/\omega) \) was connected in parallel as the leak resistor so that the capacitor \( C_2 \) does not become overloaded. The integration circuit yielded the equation \( V_y = C_2^{-1} \int I_y(t) \ dt \). When the adjustable voltage source \( V_1 \) is set to cancel the current \( I_x \) flowing into the sample, that is, if \( V_1/R_1 = V_x/R_x \) is satisfied, then the current \( I_x \) equals the current flowing into the capacitive component of the sample \( I_x = dQ/dt = d(C_1V_x)/dt \). This gives \( V_x = V_1C_1/C_2 \).
The advantage of using the op-amp is that one can choose any value of $C_2$ (as long the condition $R_2C_2 > 1/\omega$ is satisfied) to attain a larger signal $V_x$ than possible in the case in Fig. 5A. In general, the two setups in Fig. 5 (A and B) worked well. However, because the working frequency range of our op-amp (LF356N) was between 30 Hz and 30 kHz, we used setup A above 30 kHz. For frequencies below 30 kHz, both setups A and B were used. We confirmed that the two setups yielded the same results.

The measured results of the relative dielectric constants are plotted in Fig. 5C for $f = 100$ kHz and in Fig. 5D for $f = 10$ kHz. Figure 5C shows that $V_x = V_xC_1/C_2 = DS/C_2$ is proportional to $V_x = Et$. Here, $E$ is the electric field in the sample, $D$ is the dielectric displacement, and $S$ and $t$ are the area and the thickness of the sample, respectively. Using the values $S = 0.234 \text{ mm}^2$ and $t = 0.79 \text{ mm}$, we found the relative dielectric constants $\varepsilon_1 \sim 5 \times 10^6$ (shown in the inset of Fig. 5C). Unfortunately, the sample suffered dielectric breakdown above $E \sim 100 \text{ V/cm}$, which prevented us from observing the saturation of dielectric displacement $D$ at higher electric fields as should be expected from the FE behavior. This large relative dielectric constant $\varepsilon_1 \sim 5 \times 10^6$ observed in the limit $E \rightarrow 0$ strongly implies that the system is in the FE state.

We remark that the nonlinear behavior shown in Fig. 5D, previously interpreted by Möllmann et al. (22) as evidence for the FE state, is actually not the manifestation of the FE state. Rather, it arises from the fact that the resistive component of the sample $R_s$ is strongly $E$-dependent, as shown in the inset. Because $R_s$ is nonlinear, it is not possible to compensate the current $I_s$ flowing through the resistive component $R_s$ because $V_1/R_1 = V_x/R_s$ cannot be satisfied for every $V_x$, unless $V_1$ is changed nonlinearly. Therefore, if $V_1$ is set to compensate the $R_s$ at some fixed value of $V_x$ (7 V in the case of Fig. 5D), then other parts of $V_x$ cannot be compensated. As a result, they produce a nonlinear behavior that looks like the saturation expected in the FE state. The way to avoid this is to use a higher frequency $f$ so that a larger portion of the current flows into the capacitive component $C_1$ rather than into the resistive component $R_s$. This is precisely the case shown in Fig. 5C ($f = 100$ kHz).

**SUPPLEMENTARY MATERIALS**

Supplementary material for this article is available at http://advances.sciencemag.org/cgi/content/full/3/5/e1602510/DC1

section S1. Ab initio band calculations
section S2. Field-induced anomalous Hall effect
fig. S1. Calculated k-space trajectories of Weyl nodes in Pb_{1-x}Sn_xTe ($x = 0.5$) under applied pressure in zero magnetic field.
fig. S2. Phase diagram of the Weyl phase in Pb_{1-x}Sn_xTe ($x = 0.25$) and orbit parameters.
fig. S3. Phase diagram of the Weyl phase in Pb_{1-x}Sn_xTe ($x = 0.25$) in the α-β plane with applied

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Acknowledgments

Funding: The experimental project was supported by the U.S. Army Research Office (W911NF-16-1-0116) and the Gordon and Betty Moore Foundation’s Emergent Phenomena in Quantum Systems Initiative through grant GBMF4539 (to N.P.O.). R.J.C. acknowledges NSF–Materials Research Science and Engineering Center grant DMR 1402541 (crystal growth). N.K. was supported by NSF–Partnership for Research and Education in Materials grant DMR-1205734 (calculations) and the U.S. Army of Defense Grant number W911NF-16-1-0487 for the computer cluster. Author contributions: T.L. conceived the idea of applying pressure to PbSnTe and developed the experimental program with N.P.O. The samples were grown by S.K., Q.G., and T.L. with some assistance from J.L. Analyses of the results were performed by T.L. and N.P.O. The ab initio calculations were performed by J.K. and N.K. The manuscript was written by T.L. and N.P.O. with inputs from J.K. and N.K. Competing interests: The authors declare that they have no competing interests.

Data and materials availability: All data needed to evaluate the conclusions in the paper are present in the paper and/or the Supplementary Materials. Additional data related to this paper may be requested from T.L. (liang16@stanford.edu) or N.P.O. (npo@princeton.edu).

Submitted 14 October 2016
Accepted 31 March 2017
Published 31 May 2017
10.1126/sciadv.1602510

Citation: T. Liang, S. Kushwaha, J. Kim, Q. Gibson, J. Lin, N. Kiousis, R. J. Cava, N. P. Ong, A pressure-induced topological phase with large Berry curvature in Pb$_{1-x}$Sn$_x$Te. *Sci. Adv.* **3**, e1602510 (2017).
