Be$_2$Pt: Properties of a novel pseudogapped semimetal

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We report measurements and calculations on the properties of the intermetallic compound Be$_2$Pt. High-quality polycrystalline samples show a nearly constant temperature dependence of the electrical resistivity over a wide temperature range. On the other hand, relativistic electronic structure calculations indicate the existence of a narrow pseudogap in the density of states arising from accidental approximate Dirac cones extremely close to the Fermi level. A small true gap of order $\sim$3 meV is present at the Fermi level, yet the measured resistivity is nearly constant from low to room temperature. We argue that this unexpected behavior can be understood by a cancellation of the energy dependence of density of states and relaxation time due to disorder, and discuss a model for electronic transport. With applied pressure, the resistivity becomes semiconducting, consistent with theoretical calculations that show that the band gap increases with applied pressure. We further discuss the role of Be inclusions in the samples.

I. INTRODUCTION

Intermetallic compounds involving Be have not been the subject of intensive study, in part because of the element’s toxicity. However, several recent measurements in the Be-Pt series have displayed remarkable properties. Be$_{21}$Pt$_5$ is a complex metallic alloy that crystallizes in the cubic space group $\overline{4}3m$, where polyhedral 26-atom Pt-Be clusters decorate four Wyckoff sites, resulting in a 416-atom conventional unit cell. Unlike most complex metallic alloys, this material displays superconductivity below a critical temperature of $T_c = 2.06$ K [1].

Be$_2$Pt, on the other hand, crystallizes in the same space group but into a much simpler structure with only 24 atoms per conventional unit cell. The electronic structure is usually reported as semiconducting, with a gap of 190 meV deduced from the high-temperature resistivity. This is consistent with the energy scale found within density functional theory (DFT) [2] corresponding to the excitation of electrons from the top of the valence band to a sharp peak in the conduction band. However, there is a general depletion of the density of states over a wider range, decreasing down to the Fermi level, and it is difficult to judge from the calculations presented in Ref. 2 whether a true gap exists at some lower energy scale. Experimentally, the resistivity is metallic but with a nearly temperature-independent behavior over the entire measured temperature range from 3 K - 300 K. Though this suggests that the system is a metal at the lowest energies, quantitative estimates are difficult, as the samples contains a filamentary secondary phase of Be metal. The low-temperature electrical resistivity of Be (6.4 $\times$ 10$^{-9}$ $\mu$cm) can be substantially smaller than that of Cu (3.4 $\times$ 10$^{-7}$ $\mu$cm) [3]. The existence or nonexistence of a true gap, and the origin of the extremely flat temperature dependence of the resistivity below 100 K, remain puzzles.

In this work we explore the fascinating Be$_2$Pt system in greater depth. First, using an arc melting technique, we have grown polycrystalline samples which we characterize by x-ray diffraction, resistivity, Hall effect, and specific heat measurements.

We also have performed DFT calculations for this system, focusing on the low-energy band structure near the Fermi level. The unusual structure in the DOS turns out to be due to light-mass valence and conduction bands, consisting of Pt $d$ states and Be $p$ states, that nearly touch the Fermi level and exhibit a tiny indirect band gap of order only 3 meV. This makes Be$_2$Pt the only binary, nontopological intermetallic system with calculated band gap significantly smaller than room temperature [4]. Even more intriguingly the two bands near the Fermi level provide a quasilinear DOS until nearby heavier mass bands are reached; these determine the band gap previously stated in the literature. Finally, at slightly higher energies we note the existence of doubly degenerate Weyl loops within 100 meV of the Fermi level. This suggests that electron doping with, e.g. relatively small amounts of Au, could create a system with Weyl states at the Fermi level.

Next, we provide a simple model to explain the low temperature transport, including the remarkable fact that the resistivity is nearly flat in temperature, whereas the Hall coefficient decreases rapidly with decreasing temperature. The model relies on the anomalous scattering behavior of conduction electrons from static disorder in a pseudogap state, analogous to Dirac metals like graphene, although the quasi-Dirac point in this system is accidental in nature.

Finally, we present calculations and measurements of Be$_2$Pt under pressure. DFT calculations in the $F\overline{4}3m$ structure predict that the tiny gap near the Fermi level
Further opens with pressure, with concomitant enhancement of resistivity and eventually true semiconducting behavior. This is precisely what is observed in the measurements reported here. No structural transitions are anticipated theoretically, nor does the electrical resistivity data suggest such transitions up to 30 GPa.

**II. MATERIALS CHARACTERIZATION**

We prepared polycrystalline samples of Be$_5$Pt following a strategy guided by the phase diagram of Pt-Be, which shows the phases (starting from the Be-rich side of the phase diagram) Be, Be$_5$Pt, and then possibly Be$_{21}$Pt$_5$ (or Be$_{4.2}$Pt) [1]. The Be$_{21}$Pt$_5$ phase is described [1] as superconducting (resistive onset) at $T_c = 2.06$ K. When we prepared Be$_5$Pt via arc-melting, we therefore added extra Be (which has a high vapor pressure at the elevated melting temperature) to compensate for the Be mass loss during the melting process. As long as the sample remains Be-rich after arc-melting, the x-ray characterization shows single phase cubic Be$_5$Pt structure (Fig. 2), without detectable impurity phases.

If sufficient Be is evaporated in the production process to produce a sample more Be poor than the 5:1 ratio in Be$_5$Pt, the x-ray pattern becomes much more complicated, and superconductivity (absent in the stoichiometric or super-stoichiometric Be$_5$Pt samples) with a $T_c$ resistive onset of 2.47 K is detected. We presume this is indicative of the presence of a minor amount of the Amon, et al. Be$_{21}$Pt$_5$ phase [1], although our $T_c$ onset is slightly higher. In our typical preparations of Be-rich Be$_5$Pt, the excess Be tends to form connected regions (see micrograph in Fig. 3), leading to a low temperature electrical resistivity significantly lower than ideal stoichiometric Be$_5$Pt, where according to Amon et al. [2], $\rho_0$ as $T \to 0$ is $\sim 360$ m$\Omega$-cm. In Fig. 4, we show the resistivity of a sample of Be$_5$Pt, together with the

**III. ELECTRONIC STRUCTURE**

**A. Structure and Method**

Be$_5$Pt crystallizes in the non-centrosymmetric space group $F\bar{4}3m$ (#216). There are four formula units per conventional cell. Pt, Be1 and Be2 sit at Wyckoff positions 4a, 4c and 16e respectively. The linearized augmented plane wave method, as implemented in WIEN2k [5], is used to carry out first-principles calculations. The lattice constant of Be$_5$Pt is 5.975 Å. The
TABLE I. Coordinates of Pt and Be under ambient pressure obtained from DFT structure relaxation.

| Site | x    | y    | z    |
|------|------|------|------|
| Pt   | 0.4a | 0.   | 0.   |
| Be   | 4c   | 0.25 | 0.25 | 0.25 |
| Be   | 16e  | 0.124| 0.124| 0.624|

FIG. 4. Resistivity and low temperature Hall coefficient (insert).

The calculated density of states (DOS) of Be$_5$Pt has a "pseudogap“ $E_{pg}$ of roughly 400 meV, where the DOS is strongly suppressed, and in addition, a true gap $\Delta$ of $\sim 3$ meV. Low temperature transport properties of Be$_5$Pt are therefore dominated by the states in close vicinity to the Fermi level, i.e. the states near the valence band maximum and the conduction band minimum. The valence band maximum at $(0, 0.28, 0.28)$ and its equivalent k-points are trivial $M_3$ type van Hove singularities with light effective masses $m_x = 0.27m_e$, $m_y = 0.15m_e$ and $m_z = 0.17m_e$. At the $W$ point, the lowest two unoccupied states are split by 200 meV due to spin-orbit coupling. In addition, dispersion of the lowest unoccupied conduction band near $W$ is strongly anisotropic, with relatively flat dispersion along $W \rightarrow X$ and a steep slope along $W \rightarrow K$.

Because the DOS has a sharp edge above the Fermi level, a small amount of electron doping can shift states near $W$ and $X$ below the Fermi level. In Fig. 6, we plot the band dispersions of the two lowest conduction bands near the $X$ point on the $k_x - k_y$ plane. We have chosen $(001)$ as the $X$ point. Interestingly, local band dispersions on $k_x - k_y$ plane are linear near $X$, which is in agreement with Ref. [7]. The effective Hamiltonian near $X$ can therefore be written as

$$H_D = \beta (k_x \sigma_x + k_y \sigma_y)$$  \hspace{1cm} (1)$$

$\sigma_x$ and $\sigma_y$ are Pauli matrices and $k_x/y$ are crystal momenta along conventional reciprocal lattices. As a result of the linear Dresselhaus SOC, the expectation values of $s_x$ and $s_y$ are dependent on $k_x$ and $k_y$. We compute the spin textures of the two lowest conduction bands using the WIEN2k code and find that the DFT spin textures are exactly what would be obtained from the linearized $H_D$ in Eq. (1).
FIG. 6. (a) DFT low energy dispersion of the two lowest unoccupied bands on the $k_x - k_y$ plane, i.e. the plane that’s perpendicular to the $\Gamma - X$ direction. (b) band dispersion of the two lowest unoccupied bands on the $k_x - k_z$ plane. Dresselhaus spin-orbit coupling vanishes along $\Gamma - X$ which leaves the two fold spin degeneracy intact. Spin textures of the lowest and the next lowest unoccupied bands are shown in (c) and (d).

To understand the effect of pressure on the electronic structure of Be$_5$Pt, we carry out DFT calculations of Be$_5$Pt under 5, 10, 20, 30, 40, 50, 70, 90, 110, 130 and 150 GPa. Under ambient pressure, the indirect band gap of Be$_5$Pt is only 3 meV. As pressure increases from 0 to 70 GPa, the indirect band gap goes up quickly to 78 meV. Above 70 GPa, it starts to slowly decrease with higher pressure. The pseudogap, on the other hand, increases with pressure monotonically from 0.4 eV under ambient pressure to 1.2 eV under 150 GPa.

We note that pressure has a dramatically different impact on occupied vs unoccupied states near the Fermi level. The occupied states within 0.25 eV of the Fermi level are insensitive to changes in pressure. For the unoccupied states within 1 eV above the Fermi level, pressure has the effect of transferring a significant amount of spectral weight away from the Fermi level, thereby widening the pseudogap.

It is interesting to consider what may happen to the properties of this material with a small amount of electron doping, e.g. with Au. First, we expect the electronic properties to change rather rapidly, due to the steep rise in the calculated DFT density of states on the electron doped side at ambient pressure. These calculations suggest that as little as 2% Au could change the density of states at the Fermi level by orders of magnitude. In addition, slightly more Au doping should raise the chemical potential to the $\sim 0.1$ eV level where the Weyl point would be at the Fermi surface, assuming a rigid band shift. We plan to study this doping sequence in a subsequent study.

FIG. 7. DFT calculations of (a) the indirect band gap (red) and the pseudogap (blue) of Be$_5$Pt versus pressure. (b) DOS of Be$_5$Pt under pressure.

IV. INTERPRETATION OF TRANSPORT

The rather high value of the measured resistivity of our samples is consistent with a semiconducting behavior, as claimed in Ref. [2], but the temperature dependence of the resistivity, constant over more than 100 K at low $T$, is not. Electronic structure calculations presented in Sec. III (see Fig. 5) suggest, in fact, an asymmetric pseudogap in the density of states from about $-0.35$ eV to 0.05 eV, with a peak in the unoccupied density of states at the upper edge created by a flat band. Closer to the Fermi energy, a tiny true indirect gap of about 3 meV opens. At first glance, such a pseudogap/full-gap combination might be expected to lead to a semiconducting temperature dependence of the DC transport, but we argue here that this may be misleading.

Let us assume that we can model the low energy physics by an asymmetric, very slightly gapped V-shaped density of states with a tiny true gap, $\Delta = \Delta_e + \Delta_h \sim 3$ meV, as illustrated in the schematic Figure 8. We model the electronic structure relevant for low-temperature transport with two Dirac-like bands: an electron-like band, $\epsilon_k^e = \gamma_e k$ and a hole-like one, $\epsilon_k^h = -\gamma_h k$, where $k$ is measured with respect to the near-touching point of the band and we assume $\gamma_h > \gamma_e$. 
Such a model yields to a density of state linear in energy $N(\varepsilon_k) \sim \varepsilon_k$ similar to the band structure calculations. Comparing with Fig. 8, the model discussed in this section corresponds to zero gap $\Delta_\alpha = 0$, $\alpha = e, h$, and zero chemical potential $\mu$, but it can be easily generalized to include hole doping or gapping the band, both of which are discussed in the Appendix.

FIG. 8. Cartoon of Be$_2$Pt band structure near Fermi level at ambient pressure.

Electronic transport in a typical metallic system with large nonzero density of states at the Fermi level may normally be well-described by assuming a constant carrier scattering time $\tau$; this leads to a temperature-independent resistivity and Hall coefficient. Both the band structure calculations and the experimental Hall data for this system presented here suggest that this picture is incorrect. In fact, since the density of states is strongly energy-dependent near the Fermi level, a constant relaxation time approximation is no longer valid. Let us assume that the transport at low temperatures is dominated by a small number of weakly scattering point-like defects with concentration $n_i$ and potential $u_i$. As shown in the Appendix the scattering rate from point-like weak impurities for such a model is given by [8]

$$\frac{1}{\tau_\alpha(\omega)} = 2\Sigma''(\omega) = \Gamma_\alpha^0 |\omega|,$$

(2)

where we introduced the dimensionless parameter $\Gamma_\alpha^0 = n_i u_i^2/\gamma_\alpha^2$, characterizing the scattering strength. Note that we have set both the lattice parameter $a = 1$ and the reduced Planck constant $\hbar = 1$ in this and subsequent expressions.

The longitudinal conductivity is given by the sum over the bands of the hole and electron contributions that are given by

$$\sigma^\alpha_{xx} \sim \frac{e^2}{2\pi \Gamma_\alpha^0},$$

(3)

From (3), we see that the $T$-dependence of the $H = 0$ longitudinal conductivity vanishes to leading order, as expected. Note there is no universal term in the conductivity, due to the neglect of self-consistency in the Born approximation, which is relevant only over an exponentially small temperature range. The $T$-dependence of the conductivity from inelastic scattering will of course contribute at sufficiently high temperatures, but this depends on details of the system, such as Debye frequency, phonon distribution, etc. that we do not model here.

The analysis of the Hall coefficient requires the computation of the transverse component of the conductivity tensor, $\sigma_{xy}$. Also in this case, the total conductivity is given by the sum of the electron and hole contributions. As detailed in the Appendix and discussed in [9], the cyclotron frequency $\omega_c$ for a Dirac-like electronic structure is singular at zero energy, thus the denominator $(1 + \omega_c^2/T^2)$ cannot be neglected even if the magnetic field is small. Details of the derivation can be found in the Appendix, the final result for the transverse conductivity in the $\alpha$-band reads

$$\sigma^\alpha_{xy} = \pm \frac{e^2}{2\pi \Gamma_\alpha^0} \kappa^2_\alpha \int_{-\infty}^0 d\varepsilon \frac{e^2}{\varepsilon^4 + \kappa_\alpha^4} \left( - \frac{\partial f}{\partial \varepsilon} \right),$$

(4)

where the parameter $\kappa_\alpha$ has the dimensions of energy and it is defined as $\kappa_\alpha^2 = e^2 H^2/\Gamma_\alpha^0$ with $v_\alpha = \gamma_\alpha$ the band velocity. The denominator determines the $\sigma_{xy}$ $T^2$ dependence as $T \to 0$ and $1/T^2$ as $T \to \infty$. The crossover between low and high $T$ behaviors depends on the value of $\kappa_\alpha$. Now we discuss combining the contributions of hole and electron bands. Notice that in a completely symmetric model for the Dirac bands, the system would be compensated i.e. $\sigma^h_{xy} = -\sigma^e_{xy}$ and the Hall coefficient would be zero. However, in our model in order to reproduce the particle-hole asymmetry of the density of states we assume $\gamma^h > \gamma^e$, as a consequence here $\kappa^h > \kappa^e$. The asymmetry of the Dirac bands of our model implies that the total conductivity is dominated by the hole contribution since $\gamma^h > \gamma^e$. This effect is enhanced by the $T$-dependence of the chemical potential, which moves to negative values as $T$ increases (see Appendix).

Despite the fact that $\sigma_{xy}$ increases with increasing $T$, a consistent explanation of the Hall coefficient temperature dependence reported in Fig. 4 is difficult using this model alone. This is because the Hall coefficient is given by

$$R_H = \frac{\sigma_{xy}}{H(\sigma^2_{xx} + \sigma^2_{xy})},$$

(5)

and the $T$ dependence of $R_H$ depends not only on $\sigma_{xy}$, but in principle also on $\sigma_{xx}(H)$ (see Eq.A6). Applying Eq. (5) directly with the current model dominated by the hole band, gives an $R_H$ with positive sign that increases as $T \to 0$ in contrast to the experiment. The strong $T$ dependence of $\sigma^h_{xx}(H) \sim T^4$ at low $T$ is at the root of this discrepancy. As discussed in the Appendix, the inclusion of a small gap in the model does not change the Hall coefficient $T$-behavior. However, if one assumes the Fermi level lies a few meV inside the electron band, we recover a non-negligible contribution of the electron band at low temperature. This effectively cuts off the singular behavior of $R_H$ at low temperature and, within a certain range of parameters, and can reproduce a $R_H(T)$ similar to the one experimentally observed as shown in the Appendix.
However this result requires fine tuning, which is probably unreasonable given the other uncertainties in the analysis. The main source is the existence of Be inclusions in the samples, as shown in Fig. 3. Although the precise values of the resistivity of the Be inclusions in our samples are unknown, they clearly correspond to a conductivity much larger [10, 11] than the intrinsic Be$_5$Pt material, in agreement with the conclusions of Ref. 2. If we crudely model our samples as consisting of two parallel conducting channels, we expect that $\sigma = \sigma_{\text{Be}} + \sigma_{\text{Be}_5\text{Pt}}$, with $\sigma_{\text{Be}} \gg \sigma_{\text{Be}_5\text{Pt}}$. Note $\sigma_{\text{Be}}$ is the effective conductivity of the Be conducting network. Because $\sigma_{xx}$ is also $T$-independent and smaller than $\sigma_{xy}$, we may neglect it entirely in the estimation of $R_H$, and assume $\sigma_{xz} \approx \sigma_{xy}$, quite $T$-independent over 100K, and furthermore only weakly dependent on $H$ due to its strong metallic character. On the other hand, if $\sigma_{xy}$ is not too much larger than $\sigma_{xy}$, its temperature dependence will dominate the extremely weak temperature dependence of $\sigma_{xy}$. Furthermore, while the Hall coefficient of pure hcp Be metal has a positive or negative sign according to the direction of the magnetic field perpendicular to or parallel to the basal plane[12], the former value is signifiantly larger, thereby while the Hall coefficient of pure hcp Be metal has a positive sign, like $\sigma_{xy}$, which is dominated by the light hole states. The temperature dependence of the latter dominates, however, so we conclude that for our samples,

$$R_H \approx \frac{\sigma_{xy} + \sigma_{xy}}{H(\sigma_{xy})^2} \sim 1 + cT^2,$$

where $c$ is a positive constant. This result agrees qualitatively with the measured Hall coefficient of the composite sample. If samples can eventually be prepared without the Be inclusions, the Appendix contains more detailed predictions for the expected intrinsic behavior.

V. CALCULATIONS UNDER PRESSURE

We used the Genetic Algorithm for Structure and Phase Prediction (GASP) [13, 14] to search for possible phase transitions in Be$_5$Pt under pressure at fixed composition. Two GASP searches were performed at 50 GPa and 150 GPa. The ambient pressure atomic structure, along with 20 randomly generated structures, were used to initialize the GASP searches. GASP uses a genetic algorithm to perform global optimization, minimizing the enthalpy of formation in candidate structures. The algorithm iteratively creates offspring structures from parent structures by using genetic operators like mutation or mating, corresponding to operations like adding and removing atoms or splicing two structures, respectively. Structural features or genes which tend to lower the enthalpy of a structure are promoted in later structures as the algorithm progresses.

VASP was used to relax the structures and calculate the enthalpies. The cutoff energy for the plane-wave basis set was set to 520 eV. A k-point density of 20 k-points per Å$^{-1}$ was used for all the DFT relaxations. We limit the number of atoms to 12 per unit cell across the structures generated by GASP. A stopping criterion of 600 DFT relaxations was used for both GASP searches.

Fig. 9 shows the enthalpy of structures generated by GASP at 50 GPa and 150 GPa. During the GASP searches, structures that were predicted to be more stable relaxed to structures with $F43m$ space group, which is the same as that of the ambient condition ground-state structure. This indicates that no structural phase transition is seen in PtBe5 under pressure at 50 GPa and 150 GPa. The structure with $F43m$ space group has the lowest enthalpy and thus the ambient condition ground-state structure remains the most stable structure up to 150 GPa.

The absence of pressure induced structural transitions is not surprising given that the ambient pressure structures of both Pt and Be individually exhibit a remarkable stability under pressure. Platinum remains in the ambient pressure fcc structure to at least 304 GPa [15]. The stability of fcc Pt under pressure can be attributed to the fact that its neighbor to the right in the periodic table, Au, also adopts the fcc structure. Pressure is well known to induce a transfer of s-electrons into d-states in several elements. This $s \rightarrow d$ transfer often leads to structural transitions. As $s \rightarrow d$ transfer occurs in Pt, it becomes more Au-like. However, Au is also in the fcc structure, so no structural transition occurs [16]. Beryllium remains in the ambient pressure HCP phase to at least 174 GPa [17]. In the heavier alkaline earth elements (Ca, Sr, and Ba), pressure-induced $s \rightarrow d$ transfer leads to the appearance of complex crystal structures at high pressure [18]. How-
ever, Be has no nearby $d$ states. Lithium, adjacent to Be, also has no nearby $d$ states, yet exhibits a number of complex crystal structures under relatively low pressures, due to the overlap of the 1$s^2$ core electrons. However, the 1$s^2$ core of Be (1.38 pm) is substantially smaller than that of Li (1.86 pm) \[19\], and hence core overlap will not begin to occur until much higher pressures than for Li.

VI. PRESSURE DEPENDENCE OF RESISTIVITY

For the high-pressure resistivity measurements, a micro-sized Be$_5$Pt sample (\(~40 \times 40 \times 5\) $\mu$m$^3$) was cut from a larger piece of polycrystalline sample and placed in a gas-membrane-driven diamond anvil cell (OmniDAC from Almax-EasyLab) along with a ruby (\(~10\) $\mu$m in diameter) for pressure calibration \[20\]. Two opposing diamond anvils (0.15 and 0.5 mm central flats) were used, one of which was a designer-diamond anvil (0.15 mm central flat) with six symmetrically deposited tungsten microprobes in the encapsulated high-quality homoepitaxial diamond \[21\]. A 316 stainless steel metal gasket was pre-Indented from \(~150\) to 25 $\mu$m in thickness with a hole (\(~80\) $\mu$m in diameter), which was filled with soapstone (steatite) for insulating the sample and which also served as the pressure-transmitting medium.

For the resistivity calculation, we used the van der Pauw method, (assuming an isotropic sample in the measurement plane), $\rho = \pi t R / \ln 2$, where $t$ is the sample thickness (\(~5\) $\mu$m) with a current of 1 mA. The high-pressure resistivity cell was placed inside a customized continuous-flow cryostat (Oxford Instruments). A home-built optical system attached to the bottom of the cryostat was used for the visual observation of the sample and for the measurement of the ruby manometer. The pressure was applied from \(~1\) (initial loading) to 32 GPa slowly for \(~5\) hours for the pressure-dependent resistivity measurement at room temperature and then released to each pressure (Fig. 11) for the temperature-dependent resistivity measurements in the range from \(~295\) down to 1.8 K (Fig. 12).

Figure 11 shows room-temperature resistivity data under high pressure from \(~32\) down to 2 GPa during decompression. The resistivity data during compression is not shown because lead 1 (see Fig. 11 inset), used for one of the current leads, had a short with the metal gasket, which might include additional resistance in the data other than the sample. The leads for unloading pressure are without any short. It is known that resistivity obtained from decompression provides more accuracy than from compression because sample thickness is relatively well-kept during decompression \[22\]. The resistivity of Be$_5$Pt at room temperature increases under high pressures, which indicates the band gap energy ($E_g$) also increases according to the Arrhenius relation, $\rho(T) = \rho_0 \exp(E_g/2k_B T)$ at a fixed $T$. This is consistent with the band structure calculations for greater than ambient pressure in Fig. 7, showing the band gap opens further with increasing pressures to \(~27\) GPa. The inset in Fig. 11 compares the resistivity at 5 and 291 K for selected pressures. The anomaly \(~23\) GPa in Fig. 11, which shows pressure reversing, is from the adjustment of pressure determination of the ruby manometer, whereas the discontinuities in the resistivity curve are due to the changes in pressures before and after temperature-dependent resistivity measurements.

The temperature-dependent resistivity curves of Be$_5$Pt

FIG. 10. Enthalpy difference as a function of pressure of 5 lowest enthalpy structures from GASP calculation at (a) 50 GPa (b) 100 GPa. The Enthalpy is with respect to the lowest enthalpy structure ($H_r$).
are shown in Fig. 12 for five unloading pressures at 31, 22, 11, 5.7, and 2.8 GPa, including a separate ambient pressure measurement (see Fig. 4). Remarkably, the resistivity curve at ambient pressure is nearly flat over a wide temperature range compared with the high pressure resistivity curves, as discussed above. The resistivity at 2.8 GPa begins to increase monotonically with decreasing temperature, which corresponds to a typical semiconducting behavior. With further increasing pressure, the increase in temperature-dependent resistivity gets larger and larger (see Fig. 11 inset). This enhancement in the semiconducting behavior under high pressures to 31 GPa is again in a good agreement with the DFT calculations of pressure effects on Be$_2$Pt in Sec. III. The fits of the Arrhenius equation to the high pressure resistivity curves (ln$\rho$ versus 1/T plot) are shown in the Fig. 12 inset in the temperature range from $\sim$ 227 to 294 K to calculate the band gap energy ($E_g$). The estimated $E_g$ values are $\sim$ 35, 38, 39, 43, and 32 meV at 2.8, 5.7, 11, 22, and 31 GPa, respectively, which shows a good qualitative agreement with the calculated true gaps shown in Fig. 7.

VII. CONCLUSIONS

Through a series of measurements and theoretical calculations, we have argued that the little-studied intermetallic semiconductor Be$_2$Pt is in fact an extremely unusual member of its materials class. While not superconducting like its cousin Be$_2$Pd$_5$, our electronic structure calculations suggest that at ambient pressure it is semiconducting with one of the smallest gaps of any intermetallic, an indirect gap of order 3 meV according to DFT calculations we presented here. Insulating temperature dependence is not observed in low-temperature transport, however; rather the resistivity is flat at ambient pressure over a range of roughly 100K, together with a strongly $T$-dependent Hall effect.

The calculated band structure near the Fermi level has hole and electron bands resembling Dirac cones whose extrema are accidentally nearly degenerate. In addition, there is a Weyl loop structure quite close to the Fermi level, such that a small amount of doping might allow observation of topological quantization. Here we studied the transport in the quasi-Dirac cone bands and developed a model to explain the $T$-independent resistivity together with the sign and unusual $T$ dependence of the observed Hall coefficient. Agreement with experiment requires assumptions about the influence of the Be inclusions found in current samples, however.

Calculations were performed under pressure using a genetic algorithm structural relaxation method, which failed to find any phase transitions from the ambient pressure F13m structure up to 150 GPa, consistent with resistivity measurements performed in a diamond anvil cell up to this pressure. However, the temperature dependence of the resistivity evolved significantly, consistent with the opening of the gap found in DFT calculations.
In summary, we have performed a close investigation of the properties of the intermetallic semiconductor Be$_5$Pt, and shown that it is a remarkable member of this class, primarily because of an extraordinarily small accidental gap, surrounded by a somewhat larger pseudogap feature in the density of states. Additional unusual features of the band structure include Weyl loops close to the Fermi level; we have suggested that doping the compound with a small amount of gold may allow one to bring this feature to the Fermi level.

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Appendix A: Transport

We consider a two-band model with two Dirac-like bands. For the moment, we neglect the tiny gap present in the Be$_5$Pt system, i.e. we fix $\Delta_e = \Delta_h = 0$, and further assume that $\mu = 0$ at zero temperature. The band dispersion is then $\epsilon_\alpha = \pm \gamma_\alpha k$, where $\alpha = e, h$ and $k$ is measured with respect to the touching point of the band. This will yield a linear density of states in energy $N_\alpha(\epsilon) = |\epsilon|/(\gamma_\alpha^2 \pi)$. To account for the particle-hole asymmetry of the density of states found in the band structure calculations for Be$_5$Pt we need $\gamma_h > \gamma_e$. Note that because the Dirac cone is asymmetric, the chemical potential $\mu$ depends significantly on $T$ and must be calculated self-consistently.

Assuming that the transport at low temperatures is dominated by a small number of weakly scattering point-like defects with concentration $n_i$ and potential $u$ the scattering rate reads [8]

$$\frac{1}{\tau_\alpha(\omega)} = 2\Sigma''(\omega) = 2n_i u^2 \sum_k \text{Im } G(k, \omega)$$

$$= \pi n_i u^2 \int d\epsilon N_\alpha(\epsilon) \delta(\omega + \epsilon) = \Gamma_0^\alpha |\omega|, \quad (A1)$$

where we introduced the dimensionless parameter $\Gamma_0^\alpha = n_i u^2/\gamma_\alpha^2$, characterizing the scattering strength. In this and subsequent expressions we have set both the lattice parameter $a = 1$ and the reduced Planck constant $\hbar = 1$.

The longitudinal conductivity is given by the sum of the electron and hole contribution $\sigma_{xx} = \sum_\alpha \sigma_{xx}^\alpha$ with

$$\sigma_{xx}^\alpha = \frac{e^2 v_\alpha^2}{2} \int \frac{d^2 k}{(2\pi)^2} \tau_\alpha(\epsilon_k) \left( - \frac{\partial f}{\partial \epsilon_k} \right)$$

$$= \frac{e^2 v_\alpha^2}{2} \int d\epsilon N_\alpha(\epsilon) \tau_\alpha(\epsilon) \left( - \frac{\partial f}{\partial \epsilon} \right)$$

$$= \frac{e^2 \lambda_\alpha}{2\pi \Gamma_0^\alpha}, \quad (A2)$$

where $v_\alpha = \pm \gamma_\alpha$ is the velocity for the $\alpha = e, h$ band and $\lambda_\alpha$ a numerical factor coming from the evaluation of the integral and that in our case is $\lambda_h > \lambda_e$. We recover the result quoted in the main text that shows that the $T$-dependence of the longitudinal conductivity vanishes to leading order. The total conductivity is dominated by the contribution of the holes that is in our model $\sim 9$ times larger than that of the electrons. This effect results from the strong hole-electron anisotropy of the bands that forced us to assume $\gamma_h > \gamma_e$ and pushes the chemical potential to negative value as the temperature increases.

![Graph](image)

FIG. 13. Temperature dependence of the hole and electron band contributions to $\sigma_{xx}(H)$ and $\sigma_{xy}$ for $\kappa_e = 3, 10$ K. To estimate the temperature independent term $e^2/(2\pi \Gamma_0^\alpha)$, we fix $\Gamma_0^\alpha$ such that the total longitudinal conductivity at zero field, Eq.(A2), fits the experimental value $\sigma_{xx} = 0.5 \times 10^5 (\Omega m)^{-1}$. The anisotropy of band structure, encoded in the parameters $\gamma_\alpha^2 \sim 4 \gamma_e^2$, and in the temperature shift of the chemical potential to negative values, makes the transport dominated by the hole band over the whole range of temperature. $\kappa_e^2$ acts as a cut-off for the divergence of the $\sigma_{xy}^\alpha$.

The Hall coefficient in a two band system is given by

$$R_H = \frac{\sigma_{xy}}{H \left( \sigma_{xx}^2 + \sigma_{xy}^2 \right)}, \quad (A3)$$

where $H$ is the magnetic field, $\sigma_{xx} = \sum_\alpha \sigma_{xx}^\alpha$ is the total longitudinal conductivity and $\sigma_{xy} = \sum_\alpha \sigma_{xy}^\alpha$ the transverse one. Following the same procedure as in Eq.(A2),
the transverse conductivity for each band is given by\[9] \[\sigma_{xy}^\alpha = -\frac{e^2 v_{\alpha}^2}{2} \int d\epsilon N_\alpha(\epsilon) \frac{\omega^\alpha_0(\epsilon) \tau_{xy}^\alpha(\epsilon)}{1 + \left(\omega^\alpha_0(\epsilon) \tau_{xy}^\alpha(\epsilon)\right)^2} \left(-\frac{\partial f}{\partial \epsilon}\right)\]

\[= \frac{e^2}{2\pi k_B^\alpha} \kappa_{xy}^\alpha \int_{-\infty}^{0} d\epsilon \frac{e^2}{\epsilon^4 + \kappa_{xy}^\alpha^4} \left(-\frac{\partial f}{\partial \epsilon}\right), \quad (A4)\]

Here \(\omega^\alpha_0 = eHv_{\alpha}^2/\epsilon\) is the energy dependent cyclotron frequency. It is negative for the hole band, \(\epsilon_h < 0\), and positive for the electron one, \(\epsilon_e > 0\). The parameter \(\kappa_{xy}^\alpha\) is defined such that \(\omega^\alpha_0(\epsilon)\tau_{xy}^\alpha(\epsilon) = \kappa_{xy}^\alpha / \epsilon^2\), i.e.

\[\kappa_{xy}^\alpha = \frac{eHv_{\alpha}^2}{\Gamma_0^\alpha}. \quad (A5)\]

Since \(1/\tau_{xy}^\alpha(\epsilon)\) and \(N_\alpha(\epsilon)\) vary as \(\epsilon\), the integral without the \((\omega^\alpha_0)^2\) term in the denominator is actually divergent as \(1/\epsilon^2\). Thus this term is required, unlike the ordinary Hall effect for metallic systems, even in the low field limit, and determines the \(\sigma_{xy}^\alpha \sim T^2\) dependence as \(T \to 0\). To determine the crossover between low and high-temperature behavior, we must estimate the value of \(\kappa_{xy}^\alpha\) from Eq.(A5). Notice that the T-behavior of the two bands change over different energy scales as one can see in Fig.(13) where we show the T-dependence of the transverse conductivity together with the electron and hole contributions for two representative values of \(\kappa_e\). We used \(\gamma_h \sim 4\gamma_e\), as extracted from the density of states in Fig.(5) approximated as linear as shown in the schematic of Fig.(8). As a consequence we have that \(\kappa_h \sim 4\kappa_e\), thus the low-high temperature crossover appears at lower temperature for the electron term with respect to the hole term. The sign of the transvers conductivity is positive due to the dominant contribution of the hole term.

Since in the evaluation of \(\sigma_{xy}^\alpha\) we account for the full magnetic field dependence, i.e. we retain the full denominator in Eq.(A4), when computing the Hall coefficient via Eq.(A3), we need to use the same approximation for the field-dependent longitudinal conductivity \(\sigma_{xx}^\alpha\), i.e.

\[\sigma_{xx}^\alpha(H) = -\frac{e^2 v_{\alpha}^2}{2} \int d\epsilon N_\alpha(\epsilon) \frac{\tau_{xx}^\alpha(\epsilon)}{1 + \omega^\alpha_0^2(\epsilon) \tau_{xx}^\alpha(\epsilon)} \left(-\frac{\partial f}{\partial \epsilon}\right)\]

\[= \frac{e^2}{2\pi k_B^\alpha} \int_{-\infty}^{0} d\epsilon \frac{e^4}{\epsilon^4 + \kappa_{xx}^\alpha^4} \left(-\frac{\partial f}{\partial \epsilon}\right), \quad (A6)\]

whose temperature-dependence is shown in Fig.(13) for the same values of \(\kappa_{xx}\) used in the \(\sigma_{xy}\) calculation. It is evident that the total contribution of both the longitudinal and transverse conductivities come essentially form the hole band regardless of the value of \(\kappa_{xx}\). The strong anisotropy of the Dirac cone considered here reduces the two-band model to a single hole-like band model. As a consequence, the Hall coefficient reduces to \(R_H \sim \sigma_{xx}^h/(\sigma_{xy}^h)^2 + (\sigma_{xx}^h)^2\), that regardless of the exact value of the \(\kappa_{xx}\) parameter used, present a divergent behavior as \(T \to 0\) is approached, see dotted lines in Fig.(14). The anomalous temperature dependence of \(\sigma_{xx}(H) \sim T^\alpha\) at low \(T\) is at the root of this behavior in the current model.

The inclusion of a small gap in the model, does not change qualitatively the low-temperature behavior of the conductivities and of the Hall coefficient. This new energy scale could change the relative weight of the bands especially if \(\kappa_{xx}\) is of the same order of the gap. However, this effect is small with respect the suppression of the electron band contribution due to the strong temperature dependent chemical potential shift to negative values that makes the physics still dominated by the hole-like band over the whole temperature range.

An effective parameter that crucially affects the temperature dependence of the Hall coefficient is, instead, the doping. In fact, if we assume \(\mu(T = 0) > 0\), such that the Fermi level at zero temperature lays at the edge of the electron band, or further inside the band, we recover a not negligible contribution of the electron band at very low \(T\) that effectively cuts off the divergence of the Hall coefficient at low temperature, see Fig.(14) where we show the results for a specific case with \(\Delta_e = \Delta_h = 0.5\) meV and \(\mu(T = 0) = 3.4\) meV for two different values of \(\kappa_e\). As a consequence the Hall coefficient is now increasing as \(T\) is increased up to \(\sim 20\) K as seen in experiment. Notice that the crossover between the divergent \(R_H(T)\) of the un-doped model to the \(R_H(T)\) increasing with temperature of the doped case is controlled by the position of the Fermi level at zero temperature with respect the electron band, thus it is also affected by the gap values. Moreover the values of \(\kappa_{xx}\) used in the calculation influences the range of temperature over which \(R_H\) increases, i.e. the position of the peak as shown in Fig.(14). This result thus requires fine tuning, which is probably unreasonable given the other uncertainties in the analysis. In the main text we explicitly discuss the possible role of the existence of Be inclusions in the samples.
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