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Non-trivial Berry phase in the Cd_3As_2 3D Dirac semimetal

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Abstract. We present magnetotransport measurements performed on Cd_3As_2 samples. Our results confirm the existence of 3D Dirac fermions in this material with a π Berry phase. A metal-insulator transition driven by the magnetic field is also observed for B < 1 T. Finally the in situ rotation of the sample reveals that the Fermi surface is a weakly anisotropic ellipsoid.

1. Introduction

Cadmium arsenide (Cd_3As_2) is a semiconductor which has been extensively studied from the 60's to the 80's and was well-known for its high carrier mobility. Very recently, in 2013, Wang et al. computed the band structure of this material by first-principle calculations and showed that the conduction and valence bands cross along the $\Gamma - Z$ direction at finite $k_z = \pm 0.032$ Å⁻¹ [1]. The presence of two Dirac cones makes Cd₃As₂ a robust 3D semimetal, protected by the crystal symmetry. ARPES measurements first revealed that the bulk band of Cd_3As_2 presented a linear dispersion along all three momentum directions [2]. This discovery has led to a quick renewed interest in this compound and resulted in an impressive amount of experimental breakthroughs in the space of two years : negative magnetoresistance due to chiral anomaly [3], transition to a superconducting state at GPa pressures [4], possible signatures of Weyl fermions due to the breaking of time reversal symmetry [5], etc. Here, we present preliminary results obtained by magnetotransport measurements on Cd₃As₂ samples. We confirm the existence of 3D Dirac fermions and show that the Fermi surface is not exactly spherical.

2. Temperature dependence of the longitudinal resistance

In this work, we focus on several samples cleaved from a Cd_3As_2 single crystal oriented along the [112] direction. The samples present a random shape with a non uniform thickness and are not polished intentionally. The main drawback is that we cannot access the bulk carrier concentration from the Hall voltage. However it is known that there is always a discrepancy between the Hall density and the concentration estimated from the Shubnikov-de Haas in these materials [6]. This gold wires are simply contacted with silver epoxy on top of visually flat surfaces obtained after cleavage. Four-wire measurements are carried out in either the van der

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Figure 1. Longitudinal resistance R_{xx} measured as a function of the temperature for different magnetic field values. The metallic behavior observed at B = 0 T is replaced by an insulating *T*-dependence at B = 1.5 T. The sample undergoes a metal-insulator transition in between.

Pauw geometry or in a longitudinal configuration, when all four contacts are aligned. The latter is favored in order to obtain almost symmetric longitudinal resistance $R_{xx}(B)$ curves directly. We use a standard lock-in detection technique with a low frequency ac-current of 50 μ A. The samples are placed inside a variable temperature insert surrounded by a superconducting coil of 13 T.

As the temperature is cooled down, the sample's resistivity at zero magnetic field exhibits the expected metallic behavior (Fig. 1). However we observe a metal-insulator transition as the magnetic field increases. At B = 0.6 T, the resistivity is almost independent on the temperature (for T < 100 K), and above this value, the sample behaves like an insulator. We underline that a metal-insulator transition has recently been reported in Cd₃As₂ induced by biasing a top gate [7]. Anyway the metal-insulator transition of Dirac fermions is still poorly understood and requires additional theoretical studies.

Figure 2 shows the magnetic field dependence of the longitudinal resistance R_{xx} from 0 to 13 T plotted for several temperatures up to T = 153 K. The resistance exhibits a clear positive magnetoresistance (MR) with well defined superimposed Shubnikov-de Haas (SdH) oscillations for the lowest temperatures. As T increases, the positive MR diminishes and the amplitude of the SdH oscillations fades out. The low field MR is parabolic, as illustrated by the open circles on the T = 91 K curve and becomes almost linear at high magnetic field (solid circles). The latter behavior has been observed in many topological insulators and 3D semimetals. The linear MR may arise in the presence of large mobility fluctuations in the sample or when the quantum limit is reached, and all electrons lie on the lowest Landau level.

The amplitude of the SdH oscillations normalized by the value at the lowest temperature T = 2 K is plotted vs T/B in Fig. 3. For a given magnetic field, the temperature dependence is given by the Lifshitz-Kosevitch formula, $R(T) \sim X/\sinh X$, where $X = 2\pi^2 k_B m^* T/B$. The equation fits the data nicely and provides an estimate of the effective mass of 0.04 m_0 , which is in agreement with the previously reported values in this material [8].

3. Non-trivial Berry phase in Cd_3As_2

The analysis of the SdH oscillations can give access to another important property of the carriers. Indeed, the oscillating component of the magnetoresistance is given by $\Delta \rho \propto \cos(2\pi (B_f/B + 0.5 - \phi_B/2\pi))$, where B_f is the SdH oscillations frequency and ϕ_B the Berry phase. The precise determination of the phase of the oscillations is fundamental because it





Figure 2. Magnetic field dependence of the longitudinal resistance for several temperatures. Open and closed circles show *B*parabolic and *B*-linear dependences at low and high fields respectively.

Figure 3. Normalized amplitude of the SdH oscillations plotted vs T/B. The solid line is a fit by the Lifshitz-Kosevitch formula which leads to an effective mass estimation of $m^* = 0.04 m_0$.

allows to discriminate the nature of the carriers. Classical massive fermions and relativistic Dirac fermions do not exhibit the same Berry phase. For low carrier density samples, the Fermi energy is close to the Dirac point and Dirac fermions are expected with a typical π Berry phase signature. The phase is estimated from the intercept at the origin of a Landau plot as shown in the inset of Fig. 4. The inverse field of the oscillations minima and maxima is plotted as a function of the Landau level index (integer and half-integer values, respectively). Here, the intercept is equal to 0.55, i.e. $\phi_B = 1.1\pi$. This result indicates clearly a non-trivial Berry phase and the existence of 3D Dirac relativistic fermions in our Cd₃As₂ samples.



Figure 4. Longitudinal resistance vs the magnetic field at T = 2 K. Inset : inverse field of R_{xx} min and max (open/closed circles) vs the Landau level index.

4. Anisotropic Fermi surface

Finally we measured the magnetoresistance as a function of the tilt angle by an *in situ* rotation of the samples in respect to the magnetic field. Figure 5 plots the SdH frequency, i.e. the fundamental field B_f , vs the tilt angle. The frequency is not constant but varies between 37 and 43 T. This slight variation is the signature of 3D carriers, since 2D carriers are sensitive to the perpendicular component of the magnetic field only. The data should diverge when the surface becomes parallel to the applied field at 0° and 180°, which is not the case. Furthermore, the variation of the SdH frequency indicates that the cross section of the Fermi surface perpendicular to the magnetic field is not constant vs the rotation. It means that the Fermi surface is not a sphere but a weakly anisotropic ellipsoid, which confirms the conclusions of previous works [9]. Unfortunately we have not determined the in-plane crystallographic axes at this stage and cannot reconstruct the Fermi surface precisely. The 37 – 43 T range of the SdH frequency leads to an average Fermi radius varying between 0.033 and 0.036 \mathring{A}^{-1} . We deduce a carrier concentration of ~ 1.5×10^{18} cm⁻³ in our samples.



Figure 5. Fundamental field B_f as a function of the tilt angle. The behavior reveals a 3D Fermi surface with the shape of a slightly anisotropic ellipsoid (solid line is a cosine function). The 90° angle corresponds to the magnetic field normal to the sample's surface.

5. Conclusion

Transport measurements carried out at low temperature show unambiguous signatures of 3D relativistic Dirac fermions in Cd_3As_2 single crystals. A distinct Berry phase of π is estimated from the Landau plot. Additionnally, we confirm the weak anisotropy of the Fermi ellipsoidal surface.

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