Magneto-transport and electronic structures of BaZnBi2

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Abstract
We report the magneto-transport properties and electronic structures of BaZnBi2. BaZnBi2 is a quasi-two-dimensional material with metallic behavior. Transverse magnetoresistance (MR) depends on magnetic field linearly and exhibits Shubnikov–de Haas oscillation at low temperature and high field. The observed linear MR may originate from the disorder in samples or the edge conductivity in compensated two-component systems. The first-principles calculations reveal the absence of stable gapless Dirac fermion. Combined with the trivial Berry phase extracted from the SdH oscillation, BaZnBi2 is suggested as a topologically trivial semimetal. Nearly compensated electron-like Fermi surfaces (FSs) and hole-like FSs coexist in BaZnBi2.

1. Introduction

Topological semimetals, including Dirac/Weyl/nodal line semimetals, have recently attracted much attention for their extraordinary physical properties [1–18]. In these materials, linear bands cross near the Fermi level and form Dirac/Weyl points. The emergent quasi-particles are relativistic Dirac/Weyl fermions. Typical three dimensional (3D) Dirac semimetals Cd3As2 [4–7, 19, 20] and Weyl semimetals (Nb/Ta/P/As) [8–18] have been researched deeply. Several exotic transport properties such as large linear magnetoresistance (MR), high carrier mobility, non-trivial Berry phase, and chiral anomaly have been observed in them [7, 16–20].

The Mn-based ternary 112 type compounds (Ca/Sr/Ba/Eu/Yb)MnBi2 [21–37] and (Ca/Sr/Ba/Yb)MnSb2 [38–42] have been established as Dirac materials. In particular, YbMnBi2 [36] and Sr1−xMn1−xSb2 [38] have been further suggested as hosting time reversal symmetry (TRS) breaking Weyl fermions. The Bi/Sb square net in these compounds provides an ideal platform for Dirac/Weyl fermions. Since even a single-layer Bi square net can produce Dirac point [24], it is a feasible way of searching for Dirac fermions in materials including such a Bi square net.

Large unsaturated linear MR is an interesting transport phenomena in these Mn-based 112 type Dirac materials, in which the linear MR has been attributed to the extreme quantum limit of Dirac fermions [21, 26, 32, 33, 37]. In fact, there exist various materials exhibiting linear MR, such as Ag2+xSe/Ag2+xTe [43–45], n-type narrow gap semiconductor InSb [46], graphene [47, 48], topological insulators Bi2Se3/Bi2Te3 [49–51], Dirac/Weyl semimetals [7, 17, 18], etc. Several theories have been developed to explain linear MR. Abrikosov established the quantum linear MR theory for Dirac fermions in the quantum limit, where only the lowest Landau level is occupied [52]. Parish and Littlewood provided a classical route (PL model) to linear MR, in which the inhomogeneity in disordered conductors is believed to produce linear MR [53]. Hu et al expanded the PL model to 3D and identified conductivity fluctuations as the underlying physical mechanism [54]. Kisslinger et al further pointed out that the linear MR in the PL model is induced by charge carrier density fluctuations rather than mobility fluctuations [55]. Recently, Alekseev et al proposed a new classical mechanism for linear MR in two-dimensional (2D) two-component systems [48, 36, 57]. In the model, the lateral quasi-particle flow leads to the accumulation of excess quasi-particles near the sample edges. It is believed that the interplay between bulk and edge resistances gives rise to the possibility of linear MR. The mechanism is not only...
suitable for charge neutrality (compensated) two-component systems, but is also effective in systems that stay away from charge neutrality.

Motivated by the possible emergence of Dirac fermions in BaZnBi$_2$, we synthesized single crystals of BaZnBi$_2$ and studied the magneto-transport properties. The MR depends on the field linearly and angle-dependent MR reveals the two-fold symmetry of the Fermi surface in BaZnBi$_2$. Shubnikov–de Haas (SdH) oscillations can be observed clearly at low temperature and high field. However, the Landau level index fan diagram yields a trivial Berry phase and the first-principles calculations indicate the absence of stable gapless Dirac fermion and the coexistence of electron-like and hole-like Fermi surfaces (FSs) in BaZnBi$_2$. Although the structure of BaZnBi$_2$ contains single-layer Bi square net, it is suggested to be a topologically trivial material by considering the trivial Berry phase and band structures from first-principles calculations.

2. Experimental methods and crystal structure

Single crystals of BaZnBi$_2$ were grown from Bi flux. Ba, Zn and excess Bi were placed in a crucible and sealed in a quartz tube with a ratio of Ba:Zn:Bi = 1:1:6. The quartz tube was heated to 1000 °C, held there for 15 h, and cooled to 370 °C at a rate of 2 °C/h, then the excess Bi flux was removed by centrifugation. Once the samples were cooled to room temperature, silver plate-shaped crystals were obtained. The crystals can be cleaved easily. Elemental analysis was performed using energy dispersive x-ray spectroscopy (Oxford X-Max 50). The determined atomic proportion was consistent with the composition of BaZnBi$_2$ within instrumental error.

Single crystal and powder x-ray diffraction (XRD) patterns were collected from a Bruker D8 Advance x-ray diffractometer using Cu $K_{\alpha}$ radiation. TOPAS-4.2 was employed for the refinement. Resistivity measurements were performed on a Quantum Design physical property measurement system (QD PPMS-14T). The electronic structure of BaZnBi$_2$ was studied by using first-principles calculations. The projector augmented wave method [58, 59] as implemented in the VASP package [60–62] was used to describe the core electrons. For the exchange-correlation potential, the generalized gradient approximation of the Perdew–Burke–Ernzerhof formula [63] was adopted. The kinetic energy cutoff of the plane-wave basis was set to be 360 eV. A $20 \times 20 \times 20$ k-point mesh was utilized for Brillouin zone (BZ) sampling and the Fermi surface was broadened by a Gaussian smearing method with a width of 0.05 eV. The electronic structures were calculated both without and with the spin–orbital coupling (SOC) effect. The Fermi surfaces were studied by using the maximally localized Wannier function [64, 65] method and the carrier concentrations were analyzed based on the information of Fermi surface volumes. As shown in figure 1(a), BaZnBi$_2$ is isostructural with Sr/Ba/EuMnBi$_2$. BaZnBi$_2$ is comprised of alternating ZnBi and BaBi layers [66]. In the ZnBi layer, each Zn atom is surrounded by four Bi atoms, which form ZnBi$_4$ tetrahedra. In the BaBi layer, Bi atoms are separated and form a square net. Figures 2(a) and (b) show the powder and single crystal XRD patterns of BaZnBi$_2$, respectively. The powder diffraction pattern was refined by TOPAS and could be well indexed in the I4/mmm space group. The determined lattice parameters are $a = b = 4.854(2)$ Å and $c = 22.011(8)$ Å, in agreement with previously published data [66]. The single crystal XRD pattern indicates that the plane is normal to the c axis of the crystal. In consideration of the extinction phenomenon induced by the limits of crystal symmetry, only the reflections with $h + k + l = 2n$ ($n$ is an integer) are allowed. However, the observation of odd-number reflections is universal for the samples, which may come from lattice distortion or Zn deficiency.

Figure 1. (a) The crystal structure of BaZnBi$_2$. (b) The definition of polar angle $\theta$ and azimuthal angle $\varphi$. 

| $a$ | $b$ | $c$ |
|---|---|---|
| 4.854(2) Å | 4.854(2) Å | 22.011(8) Å |
3. Results and discussions

As shown in figure 3(a), the in-plane resistivity $\rho_{ab}(T)$ exhibits metallic behavior, and an external magnetic field can slightly enhance the resistivity. The MR nearly disappears when the temperature increases above 100 K. Figure 3(b) shows the magnetic field dependence of in-plane MR at different temperatures. According to
classical theory, the MR follows a quadratic \( H \) dependence and reaches saturation at high field. However, in BaZnBi\(_2\), MR increases linearly and has no sign of saturation up to 14 T. The critical point \( H_c \) of the crossover from quadratic to linear dependence on \( H \) is very small (at 2.2 K, \( H_c \approx 0.43 \) T, not presented here). The origin of the linear MR will be discussed below. The Kohler plot of BaZnBi\(_2\) is displayed in the inset of figure 3(b).

According to the Kohler’s rule \( MR = F(H/\rho_0) \) (\( \rho_0 \) is the resistivity under zero field), MR measured at different temperatures can be expressed solely as a function of \( H/\rho_0 \) if there is a single scattering time in the material. It is clear that the curves do not fall into one curve. The violation of Kohler’s rule indicates that there is more than one type of carrier in BaZnBi\(_2\) [67], which has also been confirmed by our first-principles calculations.

When a metal is in the magnetic field, the Lorentz force affects the momentum components of the carriers in the plane perpendicular to the field, consequently the MR is partially determined by the mobility in this plane. For a quasi-2D material, the carriers will only respond to the magnetic field component \( H \parallel ab \). Figure 3(c) shows the angle-dependent in-plane resistivity \( \rho_{ab}(\theta) \) under different magnetic fields (\( \varphi \) was fixed at 90°). When the magnetic field is parallel to the \( c \) axis (\( \theta = 0^\circ, 180^\circ, 360^\circ \)), resistivity has a maximum value. With the increase in the polar angle \( \theta \), the resistivity decreases gradually and reaches the minimum value when the magnetic field is parallel to the \( ab \) plane (\( \theta = 90^\circ, 270^\circ \)). The curves follow the function of \( \cos \theta \) very well, as fitted in the figure (red lines). The behavior of the angle-dependent in-plane resistivity suggests the dominance of the quasi-2D FS in BaZnBi\(_2\). Figure 3(d) shows the polar plot for \( \rho_{ab}(\theta) \), which exhibits the two-fold symmetry of the Fermi surface clearly.

Figure 4(a) shows the resistivity of BaZnBi\(_2\) as a function of field. SdH oscillation was observed at low temperature and high field. Figure 4(b) plots the oscillation amplitude \( \Delta \rho_{ab} = \rho_{ab} - \rho_{ab} \) against the reciprocal of the magnetic field \( 1/|H| \). A main oscillation frequency \( F = 178 \) T is identified from the fast Fourier transformation (FFT) spectra (figure 4(c)). Another weak frequency 251 T can also be seen from the spectra, which may be contributed by the larger hole-like FS. We analyze the principal frequency 178 T as follows. According to the Onsager relation \( F = (\phi_0/2\pi^2)A = (h/2\pi)eA \), the cross-sectional area \( A \) of the FS normal to the magnetic field is \( 1.7 \times 10^{-3} \) Å\(^2\). The Fermi wave vector is \( k_F = 0.07 \) Å\(^{-1}\) by assuming a circular cross section. The amplitude of the SdH oscillation can be described using Lifshitz–Kosevich (L–K) formula,

\[ A = \frac{\alpha}{2\pi^2} \left( \frac{\hbar}{m^*} \right)^2 \left( \frac{eB}{m^*} \right) \]

which yields the effective cyclotron resonant mass.
by the Lifshitz–Onsager quantization rule 

\[ A(\hbar/2\pi e\hbar) = n + 1/2 - \beta - \delta. \]

Figure 5. The band structures of BaZnBi2 calculated (a) without and (b) with the SOC effect. (c) Total and local density of states calculated with the SOC effect.

\[ \Delta \rho \propto \frac{\lambda T}{\sinh(\lambda T)} e^{-\lambda T D} \cos\left[ 2\pi \times \left( \frac{F}{H} - \frac{1}{2} + \beta + \delta \right) \right] \]

where \( \lambda = (2\pi^2 k_B m^* / (\hbar e\hbar)) \) and \( T_D \) is the Dingle temperature. \( 2\pi\beta \) is the Berry phase. \( \delta \) is a phase shift with the value of \( \delta = 0 \) (or \( \pm 1/8 \)) for the 2D (or 3D) system. The temperature dependence of the relative FFT amplitude can be well fitted based on the thermal factor 

\[ R_T = (\lambda T) / \sinh(\lambda T) \]

in L–K formula, as shown in the inset of figure 4(c). The cyclotron effective mass yielded by the fitting is \( m^* = 0.18 m_e \). According to the relations \( v_F = \hbar k_F / m^* \) and \( m^* = E_0 / v_F^2 \), the Fermi velocity \( v_F = 4.7 \times 10^5 \) m s\(^{-1}\) and Fermi energy \( E_F = 0.226 \) eV can also be obtained. Figure 4(d) shows \( 1/H \) as a function of Landau index \( n \). The Landau index \( n \) is related to \( 1/H \) by the Lifshitz–Onsager quantization rule 

\[ A(h/2\pi e\hbar) = n + 1/2 - \beta - \delta. \]

Considering the dominant 2D Fermi surface in BaZnBi2, the value of \( \delta \) is close to zero. So, the intercept (the lower inset in figure 4(d)) of the linear fit gives a Berry phase \( 2\pi\beta = 1.82\pi \). As is well known, the Berry phase is usually 0 or \( 2\pi \) in normal metals with a trivial parabolic dispersion relation, and the non-trivial \( \pi \) Berry phase is a transport characteristic for materials with gapless Dirac linear dispersion. The value of \( 2\pi\beta \) in BaZnBi2 is far from the non-trivial value \( \pi \), indicating BaZnBi2 is possibly a normal metal. Fitting the oscillation with the L–K formula also produces the trivial Berry phases for both 178 T and 251 T frequencies although the 251 T frequency contributes little to the oscillation. Moreover, the trivial topological property of the corresponding FS can be concluded from the first-principles calculations (see below). The upper inset in figure 4(d) shows the semilog plot of 

\[ D = \Delta \rho H \sinh(\lambda T) \]

versus \( 1/H \) at 2.2 K. The fitted Dingle temperature \( T_D \) is 11.2 K, corresponding to a carrier lifetime \( \tau_0 = \hbar / (2\pi k_B T_D) = 1.08(5) \times 10^{-13} \) s and quantum mobility \( \mu_0 = e\tau_0 / m^* = 1047 \) cm\(^2\)V\(^{-1}\)s\(^{-1}\).

Considering that the magnetic field is not high enough to drive the system into its quantum limit, the band structures of BaZnBi2 were studied by using first-principles calculations. Without the SOC effect, BaZnBi2 shows many Dirac points around the Fermi level (figure 5(a)) along the high-symmetry \( \Gamma–X, P–N, M–Z, \) and \( \Gamma–Z \) paths in the BZ (figure 6(c)). Considering the \( C_4 \) double group symmetry of BaZnBi2, only the Dirac points along the \( \Gamma–Z \) path would be protected when including the SOC effect, while others would open gaps. Nevertheless, once the SOC effect is included, the band structures of BaZnBi2 around the Fermi level show dramatic changes (figure 5(b)), and even the Dirac point along the \( \Gamma–Z \) path at 0.25 eV below the Fermi level disappears. This is because the states around the Fermi level are mainly contributed by Bi2 atoms (figure 1(a)), as deduced from the local density of states (figure 5(c)), and the strong SOC effect in heavy element Bi has great influence on related bands. Compared with the Mn-based 112 type Dirac materials, BaZnBi2 is diamagnetic and the TRS is retained. Since the breaking of TRS is suggested to play an important role on the formation of relativistic fermions in Sr\(_1\)Mn\(_{1-x}\)Sb\(_2\) [38] and YbMnBi\(_2\) [36], the topologically trivial characteristics of BaZnBi2 may be related to the absence of TRS breaking.

On the other hand, as shown in figure 5(b), the valence bands and conducting bands of BaZnBi2 have little overlap. The corresponding FSs of these bands are displayed in figure 6. Both the electron-like (figure 6(a)) FSs...
around the N–M path and one of the hole-like (figure 6(b)) FSs around the Γ point possess 2D characteristics, while the other hole-like FS around the Γ point exhibits a small ellipsoidal shape. By calculating the volumes of these FSs, we obtain the electron-like and hole-like carrier concentrations as \( n_e = 1.88 \times 10^{20} \text{ cm}^{-3} \) and \( n_h = 1.79 \times 10^{20} \text{ cm}^{-3} \), respectively. This indicates that BaZnBi\(_2\) is a charge-compensated semimetal [68].

The linear MR in BaZnBi\(_2\) is an interesting phenomenon. According to the theory of quantum MR proposed by Abrikosov [52], the linear MR will emerge when a system with gapless linear band dispersion enters the quantum limit, where all the carriers occupy the lowest Landau level. Quantum linear MR has been achieved in n-type InSb [46] and Bi\(_2\)Te\(_3\) nanosheets [50]. The linear MR in Mn–based 112 Dirac materials (Ca/Sr/Ba/Eu/Yb)MnBi\(_2\) is also suggested to be quantum MR [21, 26, 32, 33, 35, 37]. However, quantum MR is excluded in BaZnBi\(_2\) for the following reasons: (i) the first-principles calculations reveal the absence of stable gapless Dirac cone in BaZnBi\(_2\). Considering the trivial Berry phase extracted from the Landau level index fan diagram, BaZnBi\(_2\) is possibly not a Dirac material. (ii) The condition for quantum limit is \( n \ll (eH/\hbar)^{1/2} \), where \( n \) is the carrier concentration. Substituting \( n_e(n_h) \) into the expression, the quantum limit can only be reached when \( H \gg (\hbar/e)n^{1/3} \approx 216 \text{T}(209 \text{T}) \), which is not possible in the lab. Although the linear MR may emerge at a lower field with more than the lowest Landau level filled [46], the onset magnetic field of linear MR in BaZnBi\(_2\) is too far from the quantum limit.

The classical PL model [53] is usually used to explain the linear MR. In a 2D disordered conductor, mobility fluctuations (later modified as charge carrier density fluctuations by Kisslinger et al [55]) induce the distortion of the current path, and the mixture of the transverse Hall resistivity gives rise to a linear MR. The model has been expanded to the 3D case [54]. Hall measurements are usually performed to confirm the role of disorder in the generation of linear MR. However, the tests on Hall resistivity are not successful. It is difficult to obtain a smooth curve of the field-dependent Hall resistivity, which may be due to the small Hall resistivity caused by the nearly compensated carrier concentrations. As the samples’ residual resistivity ratio is small (RRR \( \approx 8 \)), disorder is inevitable and may contribute to the linear MR. Considering the refinement results of the powder XRD pattern, the disorder may come from the Zn deficiency.

Another classical mechanism was presented by Alekseev et al for the linear MR in 2D two-component systems [46, 56, 57]. According to the model, electron–hole recombination allows for a lateral quasi-particle flow and excess quasi-particles will accumulate near the edges of sample, the rise of edge conductivity will lead to the emergence of linear MR. At the charge neutrality point, the total resistivity \( \rho_{\text{total}} \) can be expressed as [56],

\[
\rho_{\text{total}}^{-1} = eP\mu \left[ \frac{1}{(\mu H)^2} + \frac{l_0}{W\mu H} \right]
\]

where \( P = n_e + n_h \) is the quasi-particle density, \( l_0 \) is the recombination length at zero field, \( W \) is the width of sample, and \( \mu \) is the mobility of carriers. Thus, the second term in equation (2) will be far beyond the first term in high field, so the MR exhibits linear behavior. As the electron and hole are nearly compensated \( (n_h/n_e \approx 0.95) \) in BaZnBi\(_2\), this theory is also possible in explaining the observed linear MR. Further experiments are needed to clarify the contribution of disorder and edge conductivity to the linear MR in BaZnBi\(_2\).

4. Summary

In summary, single crystals of BaZnBi\(_2\) were grown. BaZnBi\(_2\) exhibits two-fold symmetry magneto-transport properties and linear MR. SdH oscillations were observed at low temperature and high field, and the extracted Berry phase from the Landau level index fan diagram was topologically trivial. In the first-principles calculations, no gapless Dirac point was found when the SOC effect was included. The obtained carrier concentrations indicated that BaZnBi\(_2\) is a charge-compensated semimetal. The origin of linear MR was also discussed.
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