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Unconventional Hall effect induced by Berry curvature

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ABSTRACT

Berry phase and Berry curvature play a key role in the development of topology in physics and do contribute to the transport properties in solid state systems. In this paper, we report the finding of novel nonzero Hall effect in topological material $ZrTe_5$ flakes when the in-plane magnetic field is parallel and perpendicular to the current. Surprisingly, both symmetric and antisymmetric components with respect to magnetic field are detected in the in-plane Hall resistivity. Further theoretical analysis suggests that the magnetotransport properties originate from the anomalous velocity induced by Berry curvature in a tilted Weyl semimetal. Our work not only enriches the Hall family but also provides new insights into the Berry phase effect in topological materials.

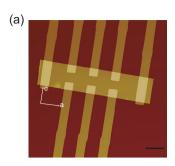
Keywords: Berry curvature, topological material, Hall effect, tilted Weyl semimetal, Berry phase effect

INTRODUCTION

The concept of Berry phase was first proposed in 1984 and has led to significant breakthroughs in physical science [1]. In recent years, Berry curvature, first discussed in the one band effective dynamics of a Bloch electron [2,3], has become an important concept in condensed matter physics [4-13]. Numerous experimental investigations show that it has to be considered in the semiclassical electronic theory as a basic ingredient. Many interesting physical phenomena can be generated by Berry curvature, such as the intrinsic anomalous Hall effect [14–18], negative magnetoresistance (MR) [19,20] and nonlinear Hall effect [21,22]. In time-reversal symmetry broken or space-inversion symmetry broken systems, the nonzero Berry curvature can generate an anomalous velocity that is transverse to the applied electric field and thus gives rise to anomalous transport currents, making an intrinsic contribution to Hall conductivity [2,4]. Besides, Berry curvature can also affect the density of states in the phase-space, which leads to the violation of Liouville's theorem for the conservation of phase-space volume [23]. As a consequence, a correction term to the density of states dependent on magnetic field and Berry curvature is

generated, which has profound effects on transport properties.

The emergence of Weyl semimetal provides a new platform to explore Berry curvature. Weyl semimetals host gapless bulk excitations described by Weyl equation and metallic Fermi arc states on the surface. As a result of band crossing between a pair of spin-non-degenerate bands, a Weyl node behaves like a magnetic monopole in momentum space and can generate divergent Berry curvature around the Weyl points [24-26]. The Berry curvature integrating over the Fermi surface enclosing a Weyl point gives a quantized topological charge, which equals the chirality of Weyl node [27]. Many interesting Berry curvature-related physical phenomena are proposed in Weyl semimetals, e.g. chiral anomaly [27,28]. Recently, it was proposed that the Berry curvature can give rise to a new type of planar Hall effect (PHE) in Weyl semimetals [29,30]. The proposed PHE appears when the electric and magnetic field are coplanar, symmetric with the magnetic field, and satisfies the angular relation: $\sigma_{vx}^{ph} =$ $\Delta \sigma \sin \theta \cos \theta$, with θ denoting the angle between the electric and magnetic fields. When coplanar electric and magnetic field are aligned in parallel and perpendicular directions, the proposed PHE signal will



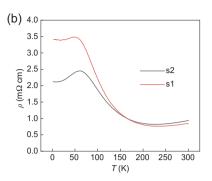


Figure 1. AFM image and ρ (T) behavior of ZrTe₅ devices. (a) AFM image of a typical ZrTe₅ device. The scale bar represents 10 μ m. (b) Resistivity of ZrTe₅ devices (s1: 300 nm thick; s2: 225 nm thick) as a function of temperature from 300 K to 2 K. A resistivity peak is detected.

vanish. The systematic experimental studies on the relation between the PHE and the magnetic field, especially on the symmetric and antisymmetric properties and the angular dependence, are still highly desired.

In this work, we present the first experimental observation of nonzero Hall effect when the in-plane magnetic field is parallel and perpendicular to the current, which is clearly revealed by systematic and reliable magnetotransport studies in topological material ZrTe₅ devices. Specifically, when the magnetic field lies in ac plane of ZrTe₅ flakes, both symmetric and antisymmetric components are observed in Hall resistivity, which cannot be explained by previous consideration of the PHE. When the in-plane magnetic field is along a axis $(B \parallel I)$ and c axis $(B \perp I)$, nonzero in-plane Hall resistivity is detected after excluding extrinsic contributions from longitudinal MR caused by slight misalignment of electrodes and inevitable projection of normal Hall resistivity at b axis. This feature is also beyond the current theoretical understanding and experimental reports on the PHE, for which the Hall signal is zero when the coplanar magnetic field and current are parallel and perpendicular [29-34]. Our theoretical analysis reveals that the tilt term in Weyl semimetal gives rise to extra contribution to the Berry curvature-induced anomalous velocity, which can explain both the symmetric and antisymmetric properties and the angular dependence of Hall signals in our measurements. Thus, our findings reveal the new properties induced by Berry curvature.

RESULTS

ZrTe₅ is a layered material, with two-dimensional sheets in *ac* plane stacking along the *b* axis, and the interlayer van der Waals coupling strength is similar to that of graphite [35]. Flat ZrTe₅ flakes can thus easily be obtained by mechanical exfoliation. Many experimental investigations have indi-

cated that ZrTe₅ can be a three-dimensional Dirac semimetal [36-39] depending on the unit cell volume of the specific crystals, and lots of interesting phenomena induced by nontrivial Berry curvature have been observed in ZrTe5, such as chiral magnetic effect [36], recently reported PHE [31] and anomalous Hall effect [40]. In this work, ZrTe₅ flakes supported by 300 nm-thick SiO₂/Si substrates were mechanically exfoliated from high quality single crystals [38]. The standard e-beam lithography followed by e-beam evaporation was used to fabricate electrodes. Figure 1(a) shows the atomic force microscope (AFM) image of a typical device for electrical transport measurements. The crystal orientation is indicated by the white arrows. ZrTe₅ flakes are often narrow in the c axis as they are easily peeled off along a axis. Refined Hall structure configuration is used to detect Hall signals of ZrTe₅ devices on ac plane. Electric current is always along a axis and homogeneously goes through the device as current electrodes $(I_+ \text{ and } I_-)$ cover the whole flake. The typical longitudinal resistivity as a function of temperature from 300 K to 2 K is shown in Fig. 1(b). Device 1 (s1, 300 nm thick) and device 2 (s2, 225 nm thick) are selected as representatives here. With temperature decreasing from 300 K to 2 K, a resistivity peak can be clearly observed in both devices. This resistivity vs. temperature (ρT) behavior is different from the resistivity saturation at low temperatures for the bulk single crystals [38], from which the flakes are exfoliated. Another feature shown in ρT behavior is that the thinner flake exhibits higher temperature of the resistivity peak, which indicates the enhancement of the metallic state in thinner flakes. Previous studies show that this may be a consequence of the energy bands shifting [41].

We further explore the magnetotransport properties of ZrTe₅ flakes in the measurement configuration when magnetic field is aligned in ac plane. Figure 2(a) shows the schematic view of the angular-dependent magnetotransport measurement configuration. The magnetic field lies in ac plane and forms an angle θ relative to the electric current. Magnetic field is along a axis for $\theta = 0^{\circ}$ $(B \parallel I)$ and along c axis for $\theta = 90^{\circ}(B \perp I)$. Figure 2(b) exhibits the longitudinal magnetoresistance (LMR) at selected angles taken in s2. Negative LMR is most evident at a axis $(B \parallel I)$, which is consistent with the prediction of chiral anomaly. Moreover, negative LMR is detected in a large regime of about $\pm\,20^\circ$, several times larger than that reported in bulk $ZrTe_5$ [36,40]. It may be due to the more precise angle control for ZrTe₅ thin flakes. Figure 2(c) shows the in-plane Hall resistivity after excluding the contribution from LMR caused by slight misalignment of electrodes, and the formula of the renormalized Hall resistivity reads ρ_{yx} =

RESEARCH ARTICLE Ge et al. | 1881

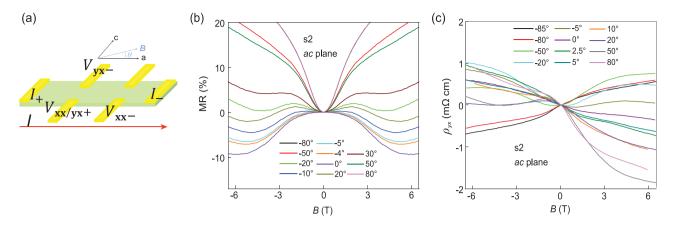


Figure 2. Angular dependence of magnetoresistance ratio and in-plane Hall resistivity in ZrTe₅ device s2. (a) Schematic structure for the angular-dependent magnetotransport measurements in ac plane. In-plane magnetic field is along a axis for $\theta=0^{\circ}$ ($B\parallel I$) and along c axis for $\theta=90^{\circ}(B\perp I)$. (b) MR behavior at selected angles. Negative LMR is detected in a large angular regime of $\pm 20^{\circ}$ and reaches maximum at $\theta=0^{\circ}$ ($B\parallel I$). (c) In-plane Hall data after subtracting ρ_{xx} caused by slight electrodes misalignment through $\rho_{yx}=\rho_{yx}^{raw}$ (B)- ρ_{xx} (B)- ρ_{xx} (B). Both symmetric and antisymmetric contributions can be observed in ρ_{yx} .

 $\rho_{yx}^{raw}(B) - \rho_{xx}(B) \cdot \frac{\rho_{yx}^{raw}(0)}{\rho_{xx}(0)}$. The raw Hall resistivity at selected angles can be found in Fig. S1. As shown in Fig. 2(c), the Hall traces exhibit both symmetric and antisymmetric components. More interestingly, nonzero Hall resistivity at $B \parallel I$ is clearly detected. This is forbidden in classical theory. The Hall resistivity should vanish at $\theta = 0^{\circ}(B \parallel I)$ even considering the current model for planar Hall resistivity in Weyl semimetals [29,30].

To understand the detected in-plane Hall signals, we separately explore the symmetric and antisymmetric components in Hall traces. The symmetric component of the in-plane Hall resistivity is obtained by the symmetrization $\rho_{yx}^{s} = \frac{\rho_{yx}(+B) + \rho_{yx}(-B)}{2}$. Figure 3(a) displays the symmetric in-plane Hall resistivity $\rho_{vx}^{s}(B)$ at selected angles in s2. As the magnetic field is increased from 0 T to 6 T, the symmetric in-plane Hall resistivity grows and finally saturates at large magnetic field at most angles. More importantly, nonzero symmetric in-plane Hall resistivity at $B \parallel I$ $(\theta = 0^{\circ})$ and $B \perp I$ $(\theta = 90^{\circ})$ can be clearly observed. The temperature dependence of the symmetric in-plane Hall resistivity $\rho_{vx}^s(B)$ at $B \parallel I$ and $B \perp I$ is shown in Fig. 3(b) and (c), respectively. At a fixed magnetic field, the absolute values of $\rho_{vx}^s(B)$ at both $B \parallel I$ and $B \perp I$ decreases as temperature increases, and finally vanishes at about 200 K. To study how in-plane Hall behavior changes with the orientation between magnetic field and current, we detect the symmetric in-plane Hall resistivity as a function of θ at various magnetic fields. Figure 3(d) illustrates the symmetric in-plane Hall resistivity taken at various magnetic fields. The same symmetrization process is carried out to remove the contribution from the antisymmetric component. At $\theta = 0^{\circ}(B \parallel I)$ and $\theta = 90^{\circ}(B \perp I)$, the nonzero symmetric in-plane Hall resistivity can be clearly detected, which is in good consistence with the Hall results in Fig. 3a.

To obtain intrinsic antisymmetric in-plane Hall resistivity, we carried out angular-dependent magnetotransport measurements in ac plane of ZrTe₅ device s2 in a triple axes vector magnet. Figure 4(a)gives the antisymmetric in-plane Hall resistivity at selected angles taken at 1.1 K. The magnetic field lies in ac plane and is tilted away from the a axis $(\theta = 0^{\circ})$. We define antisymmetric in-plane Hall resistivity as $\rho_{yx}^{as} = \frac{\rho_{yx}(+B) - \rho_{yx}(-B)}{2}$ to remove the contribution from the symmetric component. In low magnetic field region between -0.7 T and 0.7 T, linear behavior is observed at all angles. Nonzero antisymmetric in-plane Hall resistivity is detected at both $\theta = 0^{\circ}(B \parallel I)$ and $\theta =$ $90^{\circ}(B \perp I)$. We solely display the antisymmetric in-plane Hall resistivity near $B \parallel I$ and $B \perp I$ in Fig. 4(b) and (c) for clarity. As a comparison, Fig. S3 shows the antisymmetric in-plane Hall resistivity measured in Physical Property Measurement System (PPMS) after the same antisymmetrization process. Hall resistivity in the same magnetic field region from -0.7 T to 0.7 T is exhibited in Fig. S3(b), which is consistent with data in Fig. 3. Figure 4(d) and (e) shows temperature dependence of antisymmetric in-plane Hall resistivity $\rho^{as}_{yx}(B)$ at $B \parallel I$ and $B \perp I$. A linear $\rho^{as}_{yx}(B)$ behavior is clearly obtained. In low temperature regime, Hall resistivity at fixed magnetic fields slightly decreases with increasing temperature at both $B \parallel I$ and $B \perp I$.

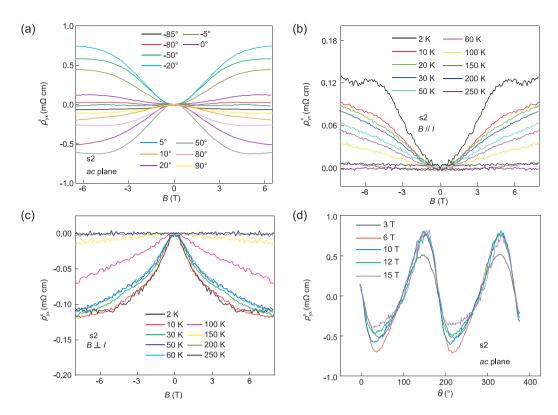


Figure 3. In-plane Hall signals detected in ZrTe₅ device s2 after symmetrization. Magnetic field lies in ac plane and is tilted away from the a axis ($\theta = 0^{\circ}$). (a) Symmetric in-plane Hall resistivity vs. B at selected angles. Symmetric in-plane Hall resistivity grows as magnetic field increases, and saturates at high magnetic fields. (b, c) Symmetric in-plane Hall resistivity vs. B at B \parallel I ($\theta=0^{\circ}$) and $B\perp$ I ($\theta=90^{\circ}$) at various temperatures. At a fixed magnetic field, the absolute values of symmetric in-plane Hall resistivity decreases as temperature increases, finally vanishing at about 200 K. (d) Symmetric inplane Hall resistivity as a function of θ at different magnetic fields (T = 2 K) with $\rho_{yx}^s = \frac{\rho_{yx}(+\beta) + \rho_{yx}(-\beta)}{2}$. All curves indicate nonzero planar Hall resistivity at $B \parallel I (\theta = 0^{\circ})$ and $B \perp I (\theta = 90^{\circ})$.

To further confirm the detected nonzero Hall signals when in-plane magnetic field is parallel and perpendicular to the current, we carry out Hall measurements in other ZrTe₅ devices too. As shown in Fig. S5, similar nonzero Hall resistivity can be observed in device s1. Therefore, in topological ZrTe₅ devices, the Hall effect does exist when in-plane magnetic field is parallel and perpendicular to the current.

The nonzero Hall resistivity detected at $B \parallel I$ or $B \perp I$ is very unusual. In fact, this unconventional behavior can be understood as the PHE in a tilted topological semimetal. Previous studies on the PHE show that the conductivities depend quadratically on the magnetic field, and the Hall signal is zero when the electric field and the magnetic field are parallel and perpendicular [29,30]. However, we theoretically find that there are linear conductivities and nonzero Hall signal at $B \parallel I$ and $B \perp I$ in the PHE of tilted Weyl semimetals, where the anomalous velocity, the chiral chemical potential and the phase volume factor all play a part. ZrTe₅ is con-

sidered as a topological semimetal in magnetic field [38]. Specifically, we investigate a low energy effective model [37] based on previous density functional theory calculation [35] and find that magnetic field drives ZrTe₅ into a tilted Weyl semimetal phase with a pair of Weyl points. (See the Supplementary Information for details.) This is not surprising, since tilt is common among Weyl semimetals, as Weyl points are typically low-symmetry points [42,43]. We performed a semiclassical calculation on the conductivities of a tilted Weyl semimetal and compare the theoretical findings with the experimental results. (See the Supplementary Information for details.) As shown in Fig. 4(f), the black circle data points are the angular dependence of observed in-plane Hall conductivity detected in a vector magnet at 1.1 K and 1 T. The in-plane Hall conductivity σ_{vx} is calculated by $\sigma_{yx} = \frac{-\rho_{yx}}{(\rho_{yx}^2 + \rho_{yx}^2)}$, here, ρ_{yx} is the in-plane Hall resistivity after subtracting ρ_{xx} caused by slight electrodes misalignment through $\rho_{yx} = \rho_{yx}^{raw} (B) - \rho_{xx}$ (B) $\frac{\rho_{yx}^{raw}(0)}{\rho_{v+}(0)}$. The red theoretical fitting curve with a RESEARCH ARTICLE Ge et al. | 1883

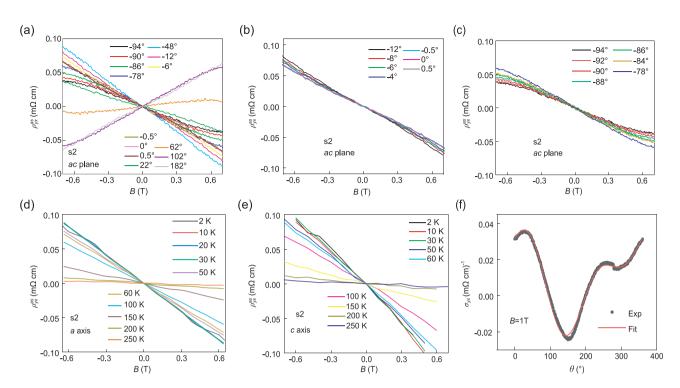


Figure 4. In-plane Hall resistivity detected in ZrTe₅ device s2 after antisymmetrization and theoretical fitting of the observed in-plane Hall conductivity. Magnetic field lies in ac plane and is tilted away from the a axis ($\theta=0^{\circ}$). (a) Antisymmetric in-plane Hall resistivity vs. B at selected angles. Linear behavior at low magnetic fields can be observed. (b, c) Antisymmetric in-plane Hall resistivity vs. B around $B \parallel I$ ($\theta=0^{\circ}$) and $B \perp I$ ($\theta=90^{\circ}$). Antisymmetric in-plane Hall signal is also apparent at both $B \parallel I$ ($\theta=0^{\circ}$) and $B \perp I$ ($\theta=90^{\circ}$). (d, e) Antisymmetric in-plane Hall resistivity versus B at $B \parallel I$ ($\theta=0^{\circ}$) and $B \perp I$ ($\theta=90^{\circ}$) at various temperatures. All Hall traces show linear behavior in low field region. (f) Theoretical fitting (red curve) of the in-plane Hall conductivity after excluding ρ_{xx} caused by slight electrodes misalignment.

set of reasonable parameters (listed in Supplementary Information) is well consistent with the experimental data [39].

The Dirac cones in ZrTe $_5$ may open a small gap Δ of the order several meV in *ab initio* calculations [26] considering the precise value of the spin orbital coupling strength. Nevertheless, in our samples $E_F >> \Delta$ is satisfied, indicating that the gap has little impact on the Berry curvature and the Fermi velocity at the Fermi surface. Therefore, our theoretical conclusion stands even considering a small gap in ZrTe $_5$.

CONCLUSION

In summary, we fabricated and measured $ZrTe_S$ devices with standard Hall bar structure. The detected Hall signals exhibit both symmetric and antisymmetric behavior when the magnetic field is in ac plane. After removing the contributions from LMR caused by slight misalignment of electrodes and projection of normal Hall with $B \parallel b$ axis, nonzero in-plane Hall resistivity is clearly obtained when in-plane magnetic field is parallel and perpendicular to the current, which is unprecedented in previous theoretical and experimental studies.

Theoretical calculation suggests that the unconventional behavior of the Hall conductivity can be understood within the semiclassical transport of the tilted Weyl semimetals, where the chiral chemical potential, the Berry curvature-induced anomalous velocity and the phase space volume correction all take part. Our discovery of nonzero in-plane Hall signals at $B \parallel I$ and $B \perp I$ not only adds a new member to the Hall effect family but also paves a new way to explore Berry phase and Berry curvature in topological materials.

METHODS

Fabrication of ZrTe₅ flake devices

The $ZrTe_5$ bulk crystals were grown as described in reference [38]. $ZrTe_5$ flakes supported by 300 nm-thick SiO_2/Si substrates were mechanically exfoliated from high quality single crystals with scotch tape. The detailed fabrication process of electrodes is described below.

 (i) Standard Electron beam lithography in a FEI Helios NanoLab 600i DualBeam System to define electrodes after spin-coating PMMA resist;

- (ii) Develop resist in an IPA: MIBK (3:1 by weight) mixture;
- (iii) Deposit Pd (6.5 nm)/Au (300 nm) in a LJUHV E-400 L E-Beam Evaporator after Ar plasma cleaning;
- (iv) Remove PMMA layers by standard lift-off process.

Transport measurements

Electrical transport measurements are conducted in a 16T-Physical Property Measurement System (PPMS-16T) from Quantum Design at 2 K and a Leiden dilution refrigerator (CF450) with a triple axes vector magnet at 1.1 K.

SUPPLEMENTARY DATA

Supplementary data are available at NSR online.

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AUTHOR CONTRIBUTIONS

J.W. conceived the research and supervised the experiments. J.G., Y. Liu, H.W., Y. Li, J.L. and T. L. performed the electrical transport measurements and analyzed the data. D. Ma, H.L. and X.C.X developed the theoretical model. J.Y. and D. Mandrus grew the bulk crystals. J.G. and Y. Li. fabricated the devices. All authors offered discussion or revisions on the manuscript.

Conflict of interest statement. None declared.

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RESEARCH ARTICLE Ge et al. | 1885

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