Magnetotransport in ZrTe5 Crystals

Maksim Andreevich Sultanov
beyondbirthday3757@gmail.com

Follow this and additional works at: https://huskiecommons.lib.niu.edu/allgraduate-thesesdissertations

Part of the Materials Science and Engineering Commons, Nanoscience and Nanotechnology Commons, and the Physics Commons

Recommended Citation
https://huskiecommons.lib.ni.edu/allgraduate-thesesdissertations/7711

This Dissertation/Thesis is brought to you for free and open access by the Graduate Research & Artistry at Huskie Commons. It has been accepted for inclusion in Graduate Research Theses & Dissertations by an authorized administrator of Huskie Commons. For more information, please contact jschumacher@niu.edu.
ABSTRACT

MAGNETOTRANSPORT IN ZrTe$_5$ CRYSTALS

Maksim A. Sultanov, MS
Department of Physics
Northern Illinois University, 2019
Zhili Xiao, Director

ZrTe$_5$ is a topological material that is predicted to have a strain or temperature - induced phase transition from a topological insulator state into a Weyl/Dirac semimetal state. In this study I find that there is insufficient evidence to support the claims for the existence of such a phase transition. I performed magnetoresistivity measurements using a Quantum Design Physical Properties Measurement System (PPMS) to measure the transverse and longitudinal resistivities at various temperatures and different strengths and orientations of the magnetic field. The measurement results were analyzed using OriginPro to determine the carrier mobility and density and to determine the temperature and magnetic field dependencies of the magnetoresistivity and magnetoconductance in the material. I conducted numerical calculations to determine the Fermi surface and the band structure of ZrTe$_5$. The calculations were performed in XCrysDen, CASTEP and the VASP package. I then compared my results with those in the literature to test the existing theories and to determine whether or not ZrTe$_5$ is a Weyl/Dirac semimetal.

I found that the magnetotransport behavior used as evidence for the existence of 2nd - order phase transition in ZrTe$_5$ could be explained by an alternative mechanism; therefore, in order to verify the categorization of the material, additional research must be performed.
MAGNETOTRANSFER IN ZrTe$_5$ CRYSTALS

BY

MAKSIM ANDREEVICH SULTANOV
©2019 Maksim Andreevich Sultanov

A THESIS SUBMITTED TO THE GRADUATE SCHOOL
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS
FOR THE DEGREE
MASTER OF SCIENCE

DEPARTMENT OF PHYSICS

Thesis Director:
Zhili Xiao
I am grateful to numerous colleagues and other individuals who have contributed their time, effort and knowledge towards this work. First, I’d like to thank my thesis advisor, Dr. Zhili Xiao, who helped me in every aspect of this work. Dr. Xiao’s mentorship allowed me to immensely grow as a researcher. I highly believe that I will remember his lessons throughout my entire life. His incredible amount of knowledge in the field of nanomaterials and the enthusiasm with which Dr. Xiao taught his class have lit a new spark of inspiration in me to perform research in the field, the result of which is this work. I am also indebted to Dr. Mikhail Semenov and Dr. Vladimir Krevchik of Penza State University for mentoring me during my undergraduate years and giving me such an excellent basis of knowledge that proved invaluable during my studies at NIU. I would also like to thank Dr. Tim Perkins, an alumnus of the NIU Chemistry and Biochemistry Department, for assisting me during a part of my research. And, of course, I would like to give thanks to my graduate - student colleagues in the NIU Physics Department for lending their vast knowledge of various fields of physics to help me improve my work and to push me to perfect it further.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>LIST OF FIGURES</th>
<th>iii</th>
</tr>
</thead>
</table>

## Chapter

1. **INTRODUCTION**
   - Topological materials ................................. 1
   - Dirac and Weyl semimetals ............................ 2
   - ZrTe$_5$ as a topological material .................... 5
   - Possible phase transition in ZrTe$_5$ .................. 7

2. **EXPERIMENTAL SETUP AND CALCULATION SOFTWARES**
   - Quantum Designs PPMS ................................. 9
   - OriginPro software ................................... 15
   - XCrysDen software .................................... 15
   - VASP package ......................................... 16
   - CASTEP ................................................ 17

3. **RESULTS AND ANALYSIS**
   - Magnetoresistivity measurements ...................... 18
   - Fermi surface and band structure .................... 27

4. **CONCLUSIONS**

REFERENCES .................................................. 38

APPENDIX: SCRIPTS USED IN PRELIMINARY ANALYSIS IN ORIGINPRO ...... 40
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Schematic image of the conduction and valence bands around the Fermi level for an insulator, a Dirac semimetal and a topological insulator.</td>
<td>2</td>
</tr>
<tr>
<td>2.</td>
<td>Schematic image of a Weyl semimetal state, with the red spheres representing Weyl nodes.</td>
<td>4</td>
</tr>
<tr>
<td>3.</td>
<td>Crystalline structure of ZrTe$_5$, its point group and the unit cell parameters.</td>
<td>6</td>
</tr>
<tr>
<td>4.</td>
<td>Plot of the longitudinal resistivity against temperature at zero magnetic field.</td>
<td>8</td>
</tr>
<tr>
<td>5.</td>
<td>Quantum Design PPMS cross-sectional schematic together with that of the probe...</td>
<td>10</td>
</tr>
<tr>
<td>6.</td>
<td>Quantum Design PPMS schematic of the probe inside.</td>
<td>11</td>
</tr>
<tr>
<td>7.</td>
<td>Gas and vacuum control scheme of Quantum Design PPMS.</td>
<td>13</td>
</tr>
<tr>
<td>8.</td>
<td>Quantum Design PPMS sample holder with several examples of chip mounts.</td>
<td>14</td>
</tr>
<tr>
<td>9.</td>
<td>Magnetic field orientation in the sample holder of the Quantum Design PPMS.</td>
<td>19</td>
</tr>
<tr>
<td>10.</td>
<td>Measurement results of resistance dependence on magnetic field magnitude for various angles of sample orientation with intervals of 10º.</td>
<td>20</td>
</tr>
<tr>
<td>11.</td>
<td>(a) Measurement results of the transverse resistance dependence on temperature for various values of the magnetic field with intervals of 0.5 T for 180º orientation of the sample. (b) Measurement results of longitudinal resistance dependence on the magnitude of magnetic field for various values of temperature with intervals of 20K for 180º orientation of the sample.</td>
<td>22</td>
</tr>
</tbody>
</table>
12. a) Longitudinal resistivity dependence on the temperature for different values of magnetic field intensity with intervals of 0.5 T. b) Transverse resistivity dependence on the temperature for different values of magnetic field intensity with intervals of 0.5 T. c) Hall factor dependence on the temperature for different values of magnetic field intensity with intervals of 0.5 T.

13. Recalculated plot of sample resistivity against temperature for different values of magnetic field with interval of 0.5 T.

14. Plotted difference between the longitudinal magnetoresistivity of the sample and the zero-field resistivity on temperature for different values of the magnetic field with intervals of 0.5 T.

15. Full band structure of the sample obtained in VASP package.

16. Total density of states of the sample obtained in VASP package.

17. Visualized Fermi surface for bands 1 to 8 for the sample obtained in VASP package and visualized with CASTEP.


19. The density of states for the experimental sample.
1. INTRODUCTION

1.1 Topological materials

Topological materials are a new type of material whose properties are highlighted and explained by topology. In mathematics, topology studies properties of objects that are invariant under smooth deformations. Materials with invariant properties under topological transformations are then classified as “topological materials”. In 2016, a team of three physicists, F. Duncan M. Haldane, Princeton University's Sherman Fairchild University Professor of Physics; J. Michael Kosterlitz of Brown University; and David J. Thouless of the University of Washington, received Nobel Prize “for theoretical discoveries of topological phase transitions and topological phases of matter”. In 1970, Michael Kosterlitz and David Thouless demonstrated that superconductivity could occur at low temperatures in thin layers and explained the mechanism that makes superconductivity disappear at higher temperatures. In 1980, Thouless explained a previous experiment with very thin electrically conducting layers in which conductance was precisely measured as integer steps, the nature of which was topological. At around the same time, Duncan Haldane discovered an explanation via topology for the properties of chains of small magnets found in some materials. A very important property of topological materials is the fact that their properties are unusually robust under physical strain or temperature shifts, which makes them attractive in the field of microelectronics, especially for the design of hazardous environment equipment.

Most common types of topological materials are topological insulators (TI) and Weyl semimetals. Topological insulators are insulators in their bulk but that have conducting states on
the surface that are protected by topology. As seen in Fig.1, in a topological insulator, similar to a regular insulator, a band gap is still present. However, the valence and the conduction band structures are different, resulting in the existence of conducting states on the surface of the material.

![Fig. 1. Schematics of the conduction and valence bands around the Fermi level for an insulator, a Dirac semimetal and a topological insulator [1].](image)

1.2 Dirac and Weyl semimetals

Another type of topological materials, as mentioned before, are Weyl semimetals. Weyl and Dirac semimetals can be viewed as three-dimensional analogs of graphene, thus generating a lot of interest in the physics community. In 1928 P. A. M. Dirac [2] proposed his famous equation, the solutions of which involved 4x4 complex matrices, allowing for both positive and negative charge solutions and for the up and down spins of fermions. In 1929, mathematician
Hermann Weyl proposed a simplified version that described massless fermions with a definite chirality (or handedness) [3]. In 1937, Ettore Majorana found a modification using real numbers, which describes a neutral particle that was its own antiparticle [4]. It was thought that this new physics would not play as important of a role in condensed matter physics as it did in particle physics. However, propagation of electrons through a periodic structure, such as a crystal lattice, leads to a variety of electronic states. As a result, the energy and angular distributions of the scattered particles are affected [2]. In some special cases, the result of this resembles the Dirac equation, with the most well-known example being graphene. Thus, in such materials, since the symmetries of free 3D space do not necessarily hold in a crystal lattice, new fermion types with no counterpart in high-energy particle physics, such as Weyl and Dirac fermions, emerge [2].

Weyl fermions are massless chiral fermions, predicted by the simplified solution to the Dirac equation. Since Dirac nodes are degenerate, it is usually said that a Dirac node is equivalent to two Weyl nodes. Weyl fermions so far have not been observed as a fundamental particle in nature. A Weyl semimetal is then a solid - state crystal with low - energy excitations that are equivalent to Weyl fermions, which can carry charge even at room temperature. Thus, a Weyl semimetal would allow for the realization of Weyl fermions in electronic systems. In a crystal of such a semimetal, the chiralities of Weyl nodes could be interpreted as topological charges. Compared to Dirac fermions in graphene or in topological insulators, Weyl fermions in Weyl semimetals are very robust and do not depend on the symmetries of the crystal lattice, with the exception being the translational symmetry.

Weyl semimetals, as opposed to topological insulators, have a linear energy to crystal momentum dispersion relation around the Weyl nodes, which are monopoles and antimonopoles
in the momentum space where the conduction and the valence bands touch. Such a dispersion relation was originally discovered for two dimensions of crystal momentum. However, the concept has since been expanded for all three special components. In the Fig. 2 we can see the visualization of the Weyl nodes in bulk of a material.

**Fig.2.** Schematic image of a Weyl semimetal state, with the red spheres representing Weyl nodes [5].

Since the Weyl nodes are separated in momentum space, parallel magnetic and electric fields can pump electrons between Weyl nodes of opposite chiralities. This process violates the
conservation of chiral charge and leads to an axial charge current, making a Weyl semimetal more conductive in an increasing magnetic field that is parallel to the electric field. Thus, negative longitudinal magnetoresistance (NLMR) is expected to be present in Weyl semimetals, which is a property that is attractive in the field of microelectronics where a quick change of resistance is useful, such as hard drive memory readout heads and various detectors that use magnetooresistance as their operating mechanism.

1.3 ZrTe₅ as a topological material

ZrTe₅ has attracted considerable attention from the scientific community throughout the years following the discovery of NLMR [6]. With the recent discoveries of numerous topological materials, researchers were using NLMR as evidence for their claims of Weyl phases in materials. However, NLMR was recently also reported for non-Weyl materials [7], thus leading many research teams to look for an alternative mechanism to support their claims.

A ZrTe₅ crystal has an orthorhombic layered structure, which could potentially be formed and studied as a 2D material due to the nature of the chains connecting the atoms. The crystal group of ZrTe₅ is Cmcm, with the dimensions of the unit cell being 4.053, 8.185 and 13.840 Å in the a, b, and c directions respectively. A visual representation of the unit cell can be seen in Fig.3. The Zr atoms form triagonal prisms of ZrTe₆, which in turn form a 1D chain of ZrTe₃ along the a axis. These prisms are coupled in the c direction via intermediate Te atom pairs, with sheets of the material in a-c planes coupled loosely by van – der - Waals forces in the b direction to form a 3D crystal. The magnitude of van – der - Waals interaction is very small, comparable
to that in graphite [6], which allows for easy cleaving in those directions. As such, both the 2D single-layer and 3D crystals of ZrTe$_5$ are of interest.

Fig. 3. Crystalline structure of ZrTe$_5$, its point group and the unit cell parameters.
1.4 Possible phase transition in ZrTe$_5$

In the search for an alternative mechanism to support the claims for existence of a Weyl phase in ZrTe$_5$, several research teams [8,9] have used a resistivity peak on the longitudinal resistivity versus temperature curves around a critical temperature of about 150K as evidence. Such a resistivity peak has been used before in HfTe$_5$ to indicate a 2$^{nd}$-order phase transition in the material, thus leading the research teams to believe that there is a temperature-induced phase transition in ZrTe$_5$ from a topological insulator state to a Weyl semimetal state. The experimental resistivity-temperature curve that was used as the evidence for a phase transition can be seen on Fig.4.

Recently, a lot of experimental studies of ZrTe$_5$ have been conducted, aiming to determine if the predicted phase transition truly occurs [8]. However, the research is extremely complicated, in no small part due to sensitivity on the lattice parameter changes and the purity of the material sample. So far, the most well-known experimental results are contradictory. Several angle-resolved photoemission spectroscopy (ARPES) studies [10] suggest a 3D Dirac semimetal band structure without a finite band gap, which coincides with the results obtained by the teams utilizing IR spectroscopy, magneto-optical and transport measurements. On the other hand, several STM studies found a band gap of 80-100 meV [8,9] and as such concluded that ZrTe$_5$ is a weak topological insulator. There is also evidence [8] for a strain-induced topological transition in ZrTe$_5$. In this research, I tested the first proposed theory and induced changes in the lattice parameters by varying temperature to see if there is a phase transition.

In this work, I studied magnetotransport in a ZrTe$_5$ crystal in an attempt to either further prove or disprove the claims for the existence of the phase transition in the material. This is done
by adopting a new approach [11] as well as comparing the obtained experimental results with other research groups [8,9]. The main argument for the presence of a 2nd-order phase transition in ZrTe₅ [8,9] was the presence of the magnetoresistivity peak at a sample-dependent critical temperature. However, I found that the peak can be explained by alternative mechanism instead, and therefore its presence is not sufficient to claim that ZrTe₅ has a phase transition.

**Fig.4.** Plot of the longitudinal resistivity against temperature at zero magnetic field. A transition is proposed at $T_p$, where the resistivity shows a peak [6].
2. EXPERIMENTAL SETUP AND CALCULATION SOFTWARES

2.1. Quantum Design PPMS

In this work, the primary measurement instrument is a Quantum Design Physical Property Measurement System (PPMS). As a measurement device, PPMS provides a flexible, automated workstation for a variety of experiments that require precise thermal and magnetic field control. It can be used to execute magnetic, electrotransport, thermoelectric measurements by itself and provides wide opportunities for modifications. Control of the sample environment includes magnetic fields up to ±9 T at a temperature range of 1.9–400 K. Temperature is measured with a typical accuracy of ±0.5 %. It can be varied with full sweep capability and slow rates from 0.01 K/min up to 12 K/min [12].

Typically, the PPMS hardware includes the dewar, the probe, the PPMS controller, a vacuum pump, and a PC. A typical schematic of the PPMS, excluding the PC necessary for operation, can be seen in Fig.5. The most interesting part of the hardware is the probe (see Fig.5), which is immersed in the liquid helium bath inside the dewar. Major components of the probe are the sample chamber, impedance assembly, baffled rods and probe head. A schematic image of the PPMS probe and the sample chamber insides can be seen in Fig.6. The sample chamber is inside the two vacuum tubes. The lower part (3.9 inches in diameter) of the sample chamber is constructed of copper in order to provide a region of uniform temperature. As shown in Fig.6, the very base of the sample chamber contains a 12-pin connector that contacts the bottom of an installed sample puck. Two thermometers and a heater are located immediately below the sample puck connector. Their proximity to the copper sample puck and the mating connector helps them
Fig.5. Quantum Design PPMS cross-sectional schematic together with that of the probe.
Fig. 6. Quantum Design PPMS schematic of the probe inside.
maintain close thermal contact with the puck and sample during experiments. The impedance assembly enables and disables the flow of helium into the cooling annulus from the dewar. The assembly consists of a narrow tube (the impedance), a heater that warms the impedance, and a thermometer that indicates when the impedance is warm. When the impedance is warm, a bubble forms inside the tube, blocking the flow of liquid helium. When the impedance heater is off, the liquid helium cools the impedance tube and flows into the cooling annulus, where it either vaporizes or fills the annulus, depending on the pressure inside the annulus. The cap at the bottom of the probe protects the impedance tube. The top part of the probe that protrudes out of the dewar is referred to as the "probe head." The probe head contains the two helium-filling ports and all the connection ports for attaching gas, vacuum, and electrical lines from the PPMS controller. The gas and pressure control scheme allows for very precise measurements and involves an oil-mist direct-drive pump that is used to control the pressure and the temperature inside the sample chamber, along with the electronic control system, a schematic of which can be seen in Fig. 7. The sample holder allows mounting chips with the samples and rotating the sample to any special orientation, permitting precise magnetotransport measurements, which is a very important feature in this study [11]. An example image of the sample holder and the chip mounts for the PPMS can be seen in Fig. 8.

PPMS also includes its own software, which is the *MultiVu* platform. It is Windows-based software that allows the user to operate and control the machine and create automation sequences to run experiments independently from the user. It also includes rudimentary graph software to view the experimental results; however, it does not in itself allow any data analysis, and therefore different software was used for that part of the work.
Fig. 7. Gas and vacuum control scheme of Quantum Design PPMS.
Fig. 8. Quantum Design PPMS sample holder with several examples of chip mounts.
2.2. OriginPro software

Origin and OriginPro are Windows-based graph and data analysis applications used for the majority of data analysis in this work. They support 2D and 3D graphing, along with such analysis methods as fitting algorithms, statistic algorithms, peak analysis, exploratory analysis and batch processing. Origin allows building various graph types, such as line plot, scatter plot, area plot, trellis plot, 3D symbol plot, 3D bar plot, 3D surface plot, etc. The curve fitting used in OriginPro is performed by a nonlinear least square fitter based on Levenberg-Maquardt algorithm. Origin is primarily a Graphical User Interface (GUI) software with an included scripting language for controlling the software (LabTalk), which is C++ based. The scripts used for data analysis in this work will be presented later in this thesis. Origin can import data files in formats such as ASCII, Excel, NI, etc.

In this work, OriginPro was primarily used for its plotting, scripting and fitting tools, which allowed us to easily analyze the experimental data and arrange them as necessary.

2.3. XCrysDen software

XCrysDen is a Windows-based software used to visualize crystalline and molecular structure. The name of the program stands for “crystalline structures and densities”, with an X because it runs under X-Window environment. It allows for display of isosurfaces and contours, which in turn can be superimposed on crystalline structures and interacted with. It also has tools for several possible analysis operations, such as visualization of Fermi surfaces, reciprocal space analysis and k-path selection in the Brillouin zone for the band structure analysis.
It should be noted that XCrysDen is free open-source software, with developers of all kinds available to modify it and write plugins for it as necessary. Notable ones include several conversion plugins from the formats of such programs as CASTEP, VASP package and others. In this work, the interactions with CASTEP and VASP package were used primarily. In particular, XCrysDen was used to visualize the Fermi surfaces for ZrTe$_5$.

2.4. VASP package

The Vienna Ab Initio Simulation Package (VASP) is used for atomic-scale materials modeling (e.g. electronic structure calculations and quantum-mechanical molecular dynamics) from first principles.

VASP computes an approximate solution to the many-body Schrödinger equation, with several options of theoretical approaches available. It can also utilize Green’s function methods and perturbation theory. It allows us to calculate the band structure for the material and export it in an image format, visualizing it. That is the feature used in this work. The advantage of using VASP instead of other conventional crystallographic software is its tremendous precision. However, it should be noted that VASP lacks a uniform GUI and is extremely difficult to work with, as it utilizes several file types that have very specific structure. Therefore, it is sometimes much easier to use software like CASTEP if such a degree of precision is not necessary.
2.5. CASTEP

CASTEP is a software also used in this work for calculation of material properties from first principles, utilizing a robust method of plane-wave basis set and pseudopotentials. The capabilities of the program include Hamiltonian methods, structural methods, molecular dynamics calculations, vibrational spectroscopy, dielectric property calculations, solid-state NMR spectroscopy, pseudopotential methods, electronic properties calculations, etc.

CASTEP in this work was primarily used for rough first calculations of band structure and k-point chain calculation that was later exported to VASP package for more precision.
3. RESULTS AND ANALYSIS

3.1 Magnetoresistivity measurements

The measurements of the longitudinal and transverse resistivity were performed using the Quantum Design PPMS. First, the sample was placed on the probe head and secured using the special sample holder. Then it was put into the sample chamber, which was later evacuated using a vacuum pump and then filled with helium gas of a few Torr for thermal exchange. The PPMS conducted a series of automated measurements using the sequence written for it, which included a full sweep of temperature from 300K to 2K. The measurements were also taken with respect to field strength, ranging from 9T to -9T and with the orientations of the sample between 180 and 90 degrees, parallel to the c axis and a-b plane of the crystal respectively. Exploring the sample with the wide range of parameters was necessary for comparing the obtained experimental results with those from other research teams.

The magnetic field orientation with respect to the position of the sample holder can be changed as a rotator in Fig.9. Magnetic field dependence of the longitudinal magnetoresistance (R-H) at a fixed temperature and various angles of sample orientation have been widely used to determine the Fermi surface of the material. Figure 10 shows results obtained for a ZrTe5 crystal at $T = 2$ K. The $R-H$ curves at high angles clearly show Shubnikov de Haas (SdH) quantum oscillations. Due to the limitation on the magnetic field strength ($\leq 9$ T), however, the $R-H$ curves do not have enough periods required for the determination of the quantum frequencies that would reveal the information on the Fermi surface. Thus, the data in Fig.10 is insufficient for the construction of the measured ZrTe5 crystal. Here I focus on the results on the temperature
Fig. 9. Magnetic field orientation in the sample holder of the Quantum Design PPMS.
Fig. 10. Measurement results of resistance dependence on magnetic field magnitude for various angles of sample orientation with intervals of 10°.
dependence of the transverse (Hall) and longitudinal resistances, which are presented in Fig.11(a) and (b), respectively. The magnetotransport measurements were also conducted using the Quantum Design PPMS, with the magnetic field applied along the c axis of the crystal and the current flowing in the plane perpendicular to it. I conducted the measurements of resistance versus temperature for different values of the magnetic field intensity. We can see the resistivity peaks in Fig.11(b), in both zero field and in the presence of magnetic fields up to 9 T. According to previous arguments [8, 9], these resistance peaks indicate phase transitions in the material.

A temperature dependence of the magnetoresistance similar to those presented in Fig.11(b) has been indeed observed in Weyl semimetal TaAs crystals [13]. It can be understood with the surface states of a Weyl semimetal, which could exhibit unusual quantum phenomena such as weak anti-localization induced by quantum interference [14]. Similar re-entrant metallic behavior was also reported to occur in graphite [15], where it has been attributed to the magnetic-field-induced occurrence of local superconductivity.

Recently, Xu et al. [11] also reported similar re-entrant metallic temperature behavior in Weyl semimetal NbP. They showed that this phenomenon can be understood using a semiclassical theory, without the need to invoke exotic mechanisms such as magnetic-field induced local superconductivity [14] or weak (anti-)localization arising from quantum interference [15]. That is, peaks in the magnetoresistance versus temperature curves are induced by the Hall effects and can disappear if the component of magnetoresistance contributed by the Hall effect is excluded.

According to Xu et al. [11], the physics is straightforward: in semiclassical theory the relationship between magnetoconductivity and magnetoresistivity is as follows:
**Fig. 11.** (a) Measurement results of the transverse resistance dependence on temperature for various values of the magnetic field with intervals of 0.5 T for 180° orientation of the sample. (b) Measurement results of longitudinal resistance dependence on the magnitude of magnetic field for various values of temperature with intervals of 20K for 180° orientation of the sample.
\[
\sigma_{xx} = \frac{\rho_{xx}}{\rho_{x}^2 + \rho_{y}^2}
\] (1)

By defining a Hall factor \( \kappa_H = (\rho_{xy}/\rho_{xx})^2 \), the relationship between \( \rho_{xx} \) and \( \sigma_{xx} \) can be written as:

\[
\rho_{xx} = \frac{1}{\sigma_{xx} (1 + \kappa_H)}
\] (2)

for a material with an ellipsoidal Fermi surface \( \sigma_{xx} = ne\mu_x/(1 + \mu_x\mu_yH^2) \). Since the mobility of electrons increases with decreasing temperature, the magnetoconductivity should decrease with decreasing temperature at high-enough magnetic fields, i.e., \( \mu_x\mu_yH^2 \gg 1 \). Xu et al. demonstrated that the Hall factor \( \kappa_H \) can have an opposite temperature dependence to that of the magnetoconductivity, resulting in a peak in the temperature dependence of the magnetoresistivity \( \rho_{xx} \). If Eq.(2) is rewritten as follows:

\[
\rho_{xx} = \frac{1}{(\sigma_{xx} + \kappa_H\sigma_{xx})}
\] (3)

we can see that the measured magnetoresistivity \( \rho_{xx} \) is determined by the magnetoconductivity \( \sigma_{xx} \) together with an additional term, \( \Delta\sigma_{xx} = \kappa_H\sigma_{xx} \), contributed by the Hall effect. Xu et al. found that in NbP crystals the curves for \( \rho_{xx}^{M} = 1/\sigma_{xx} = \rho_{xx} (1 + \kappa_H) \) versus temperature are monotonical and smooth, indicating that the resistance peaks disappear if the Hall contributions are excluded. That is, peaks in the measured magnetoresistance versus temperature curve can be induced by Hall effect, and thus they may not be associated with phase transitions.

I will use the approach of Xu et al. to analyze the data obtained from ZrTe\(_5\) crystals. My goal for this data analysis step is to utilize experimentally obtained results to make an argument for the existence of a phase transition in ZrTe\(_5\) or to see if a semiclassical theory can provide an alternative explanation for its existence.
As defined above, the Hall factor $\kappa_H = (\rho_{xy}/\rho_{xx})^2$, where $\rho_{xx} = R_{xx}wd/l$ and $\rho_{xy} = R_{xy}d$, where $w$, $d$ and $l$ are the width and thickness of the crystal and the separation between the voltage leads. The dimensions of the sample used are $w = 153.21 \, \mu m$, $d = 42.81 \, \mu m$, and $l = 1099.12 \, \mu m$. Thus $\rho_{xx}(T)$ and $\rho_{xy}(T)$ can be converted from the $R_{xx}(T)$ and $R_{xy}(T)$ in Fig.11. The associated results are presented in Fig.12(a) and (b), respectively. With the converted $\rho_{xx}(T)$ and $\rho_{xy}(T)$ in Fig.12(a) and (b), calculated the temperature-dependent Hall factors $\kappa_H = (\rho_{xy}/\rho_{xx})^2$, which are presented in Fig.12(c). The Hall factor shows a non-monotonic temperature dependence. At the low-temperature side of the resistance peak, it increases quickly with decreasing temperatures and becomes very large at low temperatures; the crossing of the $\kappa_H(T)$ curves at temperatures below 20 K is induced by SdH quantum oscillations. Thus, Hall factors can play an important role in the temperature dependence of the longitudinal magnetoresistivity $\rho_{xx}(T)$.

In order to quantify the contribution of the Hall effect, I followed the approach developed by Xu et al., i.e., to plot the $\rho_{xx}^M = 1/\sigma_{xx} = \rho_{xx}(1 + \kappa_H)$ versus temperature relationship. The results are presented in Fig.13. Compared to the $\rho_{xx}(T)$ curves in Fig.12(a), $\rho_{xx}^M(T)$ curves do not have peaks in the temperature regime where peaks occur in $\rho_{xx}(T)$ curves. Instead, they exhibit dips. This clearly indicates that the peaks in $\rho_{xx}(T)$ curves are artefacts induced by the Hall effect. On the other hand, the $\rho_{xx}^M(T)$ curves with dips in Fig.13 do differ from those of NbP, which are monotonic and smooth. An alternative explanation for the occurrence of the dips in the $\rho_{xx}^M(T)$ curves is that ZrTe$_5$ has more than one Fermi pocket. To calculate its magnetoresistivity, $\sigma_{xx}$ in Eq.(2) needs to be replaced with $\sigma_{xx} = \sum_p \sigma_{xx}^p$, where $p$ labels all the Fermi pockets. Since $\sigma_{xx}^p$ for each Fermi pocket has three free variables ($n, \mu_x, \mu_y$) with
Fig. 12. a) Longitudinal resistivity dependence on temperature for different values of magnetic field with intervals of 0.5 T. b) Transverse resistivity dependence on the temperature for different values of magnetic field intensity with intervals of 0.5 T. c) Hall factor dependence on the temperature for different values of magnetic field intensity with intervals of 0.5 T.
Fig.13. Recalculated plot of sample resistivity against temperature for different values of magnetic field with interval of 0.5T.
independent temperature dependence, thus the total $\sigma_{xx}$ and the associated $\rho_{xx}^M (= 1/\sigma_{xx})$ could have a complicated temperature dependence. In order to exclude possible influence of the zero-field resistivity, I also plotted in Fig.14 the temperature dependence of $\rho_{xx}^M - \rho_0$, where is the zero-field resistivity. Obviously, Fig.14 and Fig.13 are nearly the same. That is, $\rho_0$ does not play a significant role. In a brief summary, the experimental data was used to plot several graphs that were similar to those used as the basis of claims of phase transitions by several research teams [8, 9]. The resulting graphs can be seen on Fig. 11 and Fig. 12. My analysis outcomes are mainly presented in the Fig. 13, which shows the recalculated plot of magnetoresistivity against temperature using the semiclassical approach that I have decided to adopt. As we can see on the plot, the resistivity peak is no longer present, which indicates that there is possibly another mechanism at play. Additionally, I have plotted the difference between the magnetoresistivity and the resistivity at zero field, which exhibits a dip at the critical temperature that will counteract the peak that was used as evidence for the phase transition and will result in smooth dependence of resistivity on temperature. The resistivity dip at the critical temperature could be a potential future study subject, as there is a clear difference in the results for ZrTe$_5$ as compared to ones obtained by Xu in NbP [11].

### 3.2. Fermi surface and band structure

A preliminary analysis was performed on the data using OriginPro. First, the raw measured data array was separated with respect to parameters that would be used in further analysis, such as temperature, field intensity, angle, etc. Following that, non-data elements were removed from the array, and then the resistance was averaged for both positive and negative field
Fig. 14. Plotted difference between the longitudinal magnetoresistivity of the sample and the zero field resistivity on temperature for different values of the magnetic field with intervals of 0.5 T.
ranges. All of those actions were performed using LabTalk, which is the scripting language native to OriginPro. The scripts used can be found in the Appendix.

After analyzing the data in OriginPro, further analysis was performed using CASTEP, VASP package and XCrysDen. First, a k-mesh was constructed in CASTEP. The k-points used in this study are not reciprocal space vectors, but rather sampling points of the first Brillouin zone of the material, i.e., the specific region of reciprocal space which is closest to the gamma point. The need for k-points stems from the Bloch theorem, which states that in a periodic potential the wavefunctions have a periodic amplitude; however, it says nothing about their phase. The phase in our simulation can be assumed as periodic and repeats every three simulation cells in k_x, two cells in k_y, and every one unit in k_z. This means that if we move one simulation cell in the k_x direction, the phase would have changed by 1/3, in k_y it would have changed by 1/2, and in k_z by 1. The most general solutions for all k - phases involve integrating over all possible k; however, the solutions to Schrödinger equations change slowly with k, so the program replaces the integral over k with a sum over a grid of k-points, called a k-mesh. To figure out the cell structure and dimensions, similarity of ZrTe₅ to HfTe₅ was used in the following way: in the unit cell the atoms of Hf were replaced by Zr atoms, and an optimization algorithm was used to determine the cell parameters. Then, from the cell structure and the experimental data, we were able to get the k-path and obtain a coarse image of the band structure for the sample. The saved data was then put into VASP.

For the next step, the VASP package was used. The data from CASTEP was converted into the needed format for VASP, and the pseudopotentials for Zr and Te provided with the VASP software were used. In this step, VASP was essentially used to obtain a precise image of
the band structure for the sample, along with the data which would allow us to visualize the Fermi surface. The resulting plot of the sample band structure with the corresponding density of states can be seen in Fig. 15 and Fig. 16.

The last step of the analysis process was performed using XCrysDen. Using the data obtained from VASP package and the k-point array that we got from CASTEP, we were able to obtain and visualize the Fermi surface for the sample, along with the Brillouin zone. The resulting visualization of the Fermi surface for the sample can be seen in Fig. 17.

To analyze the Fermi surface of the sample, we used the experimental data along with the VASP package, CASTEP and XCrysDen to not only get the bar graph for the Fermi surface but also to visualize it as well using CASTEP. To do so, we started off by calculating the k-mesh for ZrTe$_5$ using the following cell parameters: point group mmm, primitive orthorhombic crystal system, and lattice parameters (a=4.053 Å, b=8.185 Å, c=13.840 Å, α=90.000°, β=90.000°, γ=104.334°). The crystal structure for ZrTe$_5$ is known to be very similar to HfTe$_5$, so in order to obtain the lattice parameters we started off with the lattice parameters for HfTe$_5$, and then we digitally replaced the Hf atoms with Zr atoms. That allowed us to perform a simulation and use XCrysDen to run a structure optimization parameter. Fig. 17 is the visualized picture of the Fermi surface for the sample.
Fig. 15. Full band structure of the sample obtained in VASP package. Fermi energy was chosen as the zero level. The resulting band structure indicates conduction and valence band overlap, which could indicate that ZrTe₅ is a semimetal.
Fig. 16. Total density of states of the sample obtained in VASP package. The dashed line represents the Fermi energy, taken as the zero level of energy, and the zero on the y axis represents the lack of states on that energy level.
Fig. 17. Visualized Fermi surface for bands 1 to 8 for the sample obtained in VASP package and visualized with CASTEP.
Comparing the Fermi surface to the one obtained in [4], we can see that the results obtained do not align well, as the surface does not appear to be elliptical, and moreover we cannot see the supposed Weyl nodes in the resulting picture that should be visible.

To conclude the analysis, the resulting data was also used to calculate the total density of states (DOS) and the band gap structure of the sample in XCrysDen to further confirm the results above. While XCrysDen is a less precise software compared to VASP package, its results are far easier to interpret, and thus are very useful. Below are the results visualized in XCrysDen. A clear direct band gap is present; however, its value does not agree with the results obtained by other research teams [8, 9], warranting further study. The resulting approximate band structure and density of states can be seen on Fig. 18 and Fig. 19. From the figures we can see that the slope of DOS is larger in the conduction band than the valence band. Such a characteristic is also found in the other works on ZrTe$_5$ [8].
Fig. 18. Band structure of the experimental sample. While greatly simplified, the band structure still indicates a slight overlap of valence and conduction bands, thus supporting the point for classification of ZrTe$_5$ as a semimetal.
Fig. 19. The density of states for the experimental sample. Comparing it to VASP results, we can see the difference around the Fermi level, which is chosen to be the zero level in this picture. Non-zero density of states around the Fermi level could be an indication that the material is a semimetal, which contradicts earlier results obtained in VASP package; however, due to the simplicity of XCrysDen, I am inclined to trust its results more.
CONCLUSIONS

From the obtained experimental results and the analysis that followed them, I conclude that the resistance peak used by other teams [8, 9] is not enough to support the claim for the strain-induced or temperature-induced topological phase transition in ZrTe$_5$. My own experimental results for the resistance do not lead to a clear conclusion on the topic of debate, the existence of phase transition into a Weyl semimetal. However, based on the experimental data, I can conclude that under the conditions present in the experiment, ZrTe$_5$ exhibits a weak topological insulator phase. As a future goal for such research, I plan to conduct more experimental research on the magnetic field dependence of the resistance at various field orientations to determine the Fermi surface of ZrTe$_5$. I will perform more systematic calculations on the change of band structure under various temperatures and fields to form a solid conclusion on the re-entrant metallic behavior in the material, as it would allow me to study the behavior in Fermi nodes in the materials and possibly see the split of Dirac cones into Weyl nodes at low temperatures.
REFERENCES


APPENDIX
SCRIPTS USED IN PRELIMINARY ANALYSIS IN ORIGINPRO
1) RH data for various angles

separate RH data with Temperature

win -a book1;

j=1;
jmax=61;
tempError=0.2;

rhname$="RHTK";
A_jj=Temp_A[jj];
string strjj$ = $(A_jj); number to string
rhname.Insert(4,strjj$); insert number to file name string
newbook % (rhname$) option:=lsname; create new workbook for the first temperature
win -a % (rhname$);
work -a 2;
work -t 2 4;
col(D)[C]$=strjj$; set comment

for(ii=1,kk=1; ii<=aa && jj<=jmax; ii++){

if(abs(A_jj-book1_C33[ii])<tempError){
col(A)[kk]=book1_C33[ii]; temperature
col(B)[kk]=book1_C3[ii]; magnetic field
col(C)[kk]=book1_C20[ii]; RXy;
col(D)[kk]=book1_C19[ii]; RXx;
kk++;
}
else {
kk=1;
jj++;
rhname$="RHTK";
A_jj=Temp_A[jj];
string strjj$ = $(A_jj); number to string
rhname.Insert(4,strjj$); insert number to file name string
newbook % (rhname$) option:=lsname; create new workbook for the first temperature
win -a % (rhname$);
work -a 2;
work -t 2 4;
//col(C)[C]$=jj;
col(D)[C]$=strjj$;
ii--;
}
}
jj=1; //first temperature;
jmax=61; //highest temperature;

for( ;jj<=jmax; ){  
    //step setting see the bottom of this for loop
    rname$="RHTK";
    A_jj=Temp_A[jj];
    string strjj$ = $(A_jj); //number to string
    rname.Insert(4,strjj$); //insert number to file name string
    win -a %rname$;

    work -a 6;
    work -t 6 4;
    work -t 9 4;

    col(E)[C]$="Temperature";
    col(F)[C]$="Field";
    strRxy$="RxyK";
    strRxy.Insert(4,strjj$); //insert number to file name string
    col(G)[C]$=strRxy$;

    col(H)[C]$="Temperature";
    col(I)[C]$="Field";
    strRxx$="RxxK";
    strRxx.Insert(4,strjj$); //insert number to file name string
    col(J)[C]$=strRxx$;

    aa=wks.col1.nRows; //find out how many rows;
    aa=aa/2;
    for(ii=1;ii<=aa;ii++){  
        col(E)[ii]=col(A)[2*ii];
        col(F)[ii]=col(B)[2*ii];
        col(G)[ii]=col(C)[2*ii];
        col(H)[ii]=col(A)[2*ii-1];
        col(I)[ii]=col(B)[2*ii-1];
col(J)[ii]=col(D)[2*ii-1];
}

int j=1; //first temperature;
int jmax=61; //highest temperature;

for ( int jj=1; jj<=jmax; jj++) {
    //step setting see the bottom of this for loop
    char rhname$="RHTK";
    A[jj]=Temp_A[jj];
    string strjj$ = $(A[jj]); //number to string
    rhname.Insert(4,strjj$); //insert number to file name string
    win -a %rhname$;
    work -a 6;
    work -t 11 4;
    work -t 14 4;

    //set comment information below
    col(K)[C]$="FieldRverse";
    strRxy$="RxyK";
    strRxy.Insert(4,strjj$); //insert number to file name string
    col(L)[C]$=strRxy$;
    strRxy$="RxyKAverage";
    strRxy.Insert(4,strjj$); //insert number to file name string
    col(M)[C]$=strRxy$;
    col(N)[C]$="FieldRverse";
    strRxx$="RxxK";
    strRxx.Insert(4,strjj$); //insert number to file name string
    col(O)[C]$=strRxx$;
    strRxx$="RxxKAverage";
    strRxx.Insert(4,strjj$); //insert number to file name string
    col(P)[C]$=strRxx$;
aa=wks.col1.nRows;//find out how many rows;
aa=aa/2;
for(ii=1;ii<=aa;ii++){
col(K)[ii]=col(F)[aa+1-ii]*(-1);
col(L)[ii]=col(G)[aa+1-ii];
col(N)[ii]=col(I)[aa+1-ii]*(-1);
col(O)[ii]=col(J)[aa+1-ii];
}//end for

//for(ii=aa+1;ii<=aa*2;ii++){
//col(K)[ii]=" ";
//col(L)[ii]=" ";
//col(N)[ii]=" ";
//col(O)[ii]=" ";
}//end for

col(M)=(col(G)(col(K))-col(L))/2;
col(P)=(col(J)(col(N))+col(O))/2;

///////set step information here
jj++;
A_ijj=Temp_A[jj];
}//end for;

2)RH data for various temperatures
///////////separate RH data with Temperature///////////
//////////separate RH data with Temperature///////////
win -a book1;
aa=wks.col2.nRows;//find out how many rows;

jj=1;
jmax=61;
tempError=0.2;
rhname$="RHTK";
A_ijj=Temp_A[jj];
string strjj$ = $A_ijj;//number to string
rhname.Insert(4,strjj$);//insert number to file name string
newbook %rhname$ option:=lsname://create new wookbook for the first temperature
win -a %rhname$;
work -a 2;
work -t 2 4;
col(D)[C]$=strjj$;//set comment

for(ii=1,kk=1; ii<=aa && jj<=jmax; ii++)
{
    if(abs(A_jj-book1_C33[ii])<tempError)
    {
        col(A)[kk]=book1_C33[ii];//temperature
        col(B)[kk]=book1_C3[ii];//magnetic field
        col(C)[kk]=book1_C20[ii];//Rxy;
        col(D)[kk]=book1_C19[ii];//Rxx;
        kk++;
    }
    else {
        kk=1;
        jj++;
        rhname$="RHTK";
        A_jj=Temp_A[jj];
        string strjj$ = $(A_jj);//number to string
        rhname.Insert(4,strjj$);//insert number to file name string
        newbook %(rhname$) option:=lsname;//create new workbook for the first temperature
        win -a %(rhname$);
    }
}

jj=1;//first temperature;
jmax=61;//highest temperature;

for( jj<=jmax; )
{
    //step setting see the bottom of this for loop
    rhname$="RHTK";
    A_jj=Temp_A[jj];
    string strjj$ = $(A_jj);//number to string
    rhname.Insert(4,strjj$);//insert number to file name string
    win -a %%(rhname$);
work -a 6;
work -t 6 4;
work -t 9 4;

col(E)[C]$="Temperature";
col(F)[C]$="Field";
strRxy$="RxyK";
strRxy.Insert(4,strjj$);//insert number to file name string
col(G)[C]$=strRxy$;

col(H)[C]$="Temperature";
col(I)[C]$="Field";
strRxx$="RxxK";
strRxx.Insert(4,strjj$);//insert number to file name string
col(J)[C]$=strRxx$;

aa=wks.col1.nRows;//find out how many rows;
aa=aa/2;
for(ii=1;ii<=aa;ii++){
  col(E)[ii]=col(A)[2*ii];
  col(F)[ii]=col(B)[2*ii];
  col(G)[ii]=col(C)[2*ii];
  col(H)[ii]=col(A)[2*ii-1];
  col(I)[ii]=col(B)[2*ii-1];
  col(J)[ii]=col(D)[2*ii-1];
}

///set step information here
jj++;
A_00=Temp_A[jj];
}//end for;

///average Rxx and Rxy of negative and positive field///
jj=1; //first temperature;
//jmax=61; //highest temperature;
for( ;jj<=jmax; ){
  //step setting see the bottom of this for loop
  rhname$="RHTK";
A_\_jj=\text{Temp}\_A[\_jj];
string \_strjj$ = $A_\_jj$;//number to string
\_rhn\_name.Insert(4,\_strjj$);//insert number to file name string
\_w\_in$ -$a$ %\(_rhn\_name$);

\_w\_ork$ -$a$ 6;
\_w\_ork$ -$t$ 11 4;
\_w\_ork$ -$t$ 14 4;

//set comment information below
col(K)[C]$ = "FieldReverse";
\_strR\_xy$ = "RxyK";
\_strR\_xy$\.Insert(4,\_strjj$);//insert number to file name string
\_col(L)[C]$ = \_strR\_xy$;
\_strR\_xy$ = "RxyKAverage";
\_strR\_xy$\.Insert(4,\_strjj$);//insert number to file name string
\_col(M)[C]$ = \_strR\_xy$;

\_col(N)[C]$ = "FieldReverse";
\_strRx\_x$ = "RxxK";
\_strR\_xx$\.Insert(4,\_strjj$);//insert number to file name string
\_col(O)[C]$ = \_strRx\_x$;
\_strRx\_x$ = "RxxKAverage";
\_strR\_xx$\.Insert(4,\_strjj$);//insert number to file name string
\_col(P)[C]$ = \_strRx\_x$;

\_aa=\_wks\.col1\.n\_Rows; //find out how many rows;
\_aa=\_aa/2;
for(ii=1;ii<=\_aa;ii++){\n   \_col(K)[ii]=\_col(F)\[aa+1-\_ii\]*(-1);
   \_col(L)[ii]=\_col(G)\[aa+1-\_ii\];
   \_col(N)[ii]=\_col(I)\[aa+1-\_ii\]*(-1);
   \_col(O)[ii]=\_col(J)\[aa+1-\_ii\];
} //end for

//for(ii=aa+1;ii<=aa*2;ii++){\n   //\_col(K)[\_ii]=" ";
   //\_col(L)[\_ii]=" ";
   //\_col(N)[\_ii]=" ";
   //\_col(O)[\_ii]=" ";
   //} //end for

\_col(M)=\(\_col(G)(\_col(K)) - \_col(L))/2;
col(P) = (col(J)(col(N)) + col(O))/2;

///////set step information here
jj++;
A_\text{jj}=\text{Temp}_A[\text{jj}];
} // end for;