Observation of Gapless Nodal-Lines in a Rare-Earth-Based Compound

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OBSERVATION OF GAPLESS NODAL LINES IN A RARE-EARTH-BASED COMPOUND

by

ROBERT SMITH

A thesis submitted in partial fulfillment of the requirements for the Honors in the Major Program in Physics in the College of Sciences and in the Burnett Honors College at the University of Central Florida Orlando, Florida

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Thesis Chair: Madhab Neupane, Ph.D.
ABSTRACT

This thesis aims to contribute to the understanding of quantum materials by employing a combination of experimental techniques, such as angle-resolved photoemission spectroscopy and magnetic and transport measurements. Further collaborative support in the form of first-principles calculations is included and discussed in tandem. In this thesis, a lanthanide-based semimetal of the ZrSiS type, is investigated. Multiple nodal lines which remain gapless are observed along the X-R direction of the Brillouin zone. We also present a nodal line that is observed further below the Fermi level and aligned in the Γ-M direction; this nodal line appears to be sensitive to light source polarization. A surface state at the X point is also observed. Finally, this thesis includes some discussion on the development of a sample growth laboratory, along with the presentation and characterization of grown Bi$_2$Se$_3$ samples. With potential applications in the fields of spintronics and novel microelectronic devices, the experimental realization and understanding of quantum materials is key to a deeper understanding of materials physics.
ACKNOWLEDGMENTS

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CHAPTER 1: INTRODUCTION

History and importance

Condensed matter physics, as a field, is exceptionally fast-paced. An astonishing number of materials with unique properties are discovered, classified, and experimentally investigated in a stream of exciting publications. Recently, the prediction and experimental discovery of novel phases of matter sparked a considerable explosion in condensed matter physics research. Combining the study of band theory, single-crystal and thin-film growth, topology, and many quantum mechanical principles, a new subfield emerged referred to as “topological materials.” Drawing on the mathematical robustness of topology, these materials exhibit exotic and novel electronic states, which were first discovered in a quantum variation of the Hall effect. In 1982 the quantum Hall effect was discovered by von Klitzing, which shed new light on semiconductor physics research as an avenue for fundamental discoveries in modern physics [1]. Von Klitzing received the Physics Nobel Prize for his discoveries not long afterward in 1985. Analyzing electronic behavior when confined to two dimensions in the presence of a strong, perpendicular, external magnetic field, a quantized Hall conductivity was observed. This realization described Hall conductance strictly in terms of the fundamental constants electronic charge $e$ and Planck’s constant $h$, $2e^2/h$, instead of a complicated amalgamation of lattice parameters, band gaps, or electronic properties specific to a material. That is, at sufficiently low temperatures and with a strong enough external magnetic field, plateaus were observed in the Hall conductivity as it took on quantized integer multiples of fundamental constants. Soon after, the exploration of topological phases expanded quickly with various classifications of electronic properties such as topological insulators (TIs) [2–4] and topological semimetals (TSMs) [5, 6]. These classifications stem from each phase’s unique topological “invariant,” distinguishing robust surface states from more mundane bulk states [7].
With the considerable attention drawn to topological materials (TMs) in recent years, applications of the observed exotic properties have already been predicted and realized experimentally. Specifically, great interest exists in applying these materials to photoelectric conversion, light harvesting, and photoelectric conversion fields of energy [8]. These developments in understanding electron spin in TIs could prove revolutionary in future electronics. More specifically, electronic applications such as spintronics and magnetoelectronics may revolutionize the future of computing [9].

Introduction to topology

In the pure mathematical sense, a topological space is simply a set paired with a topology. One may interpret a topological space as similar to a geometric space, in which a well-defined distance separates points, even if the said separation is not necessarily a numeric value. Such a notion is apparent in the case of metric spaces, a convenient example of topological spaces. From here, the study of topology is primarily concerned with the properties of objects under continuous deformation. One may understand these deformations in geometric space as stretching, squishing, twisting, and so on; the essential requirement is that no new holes are formed, nor existing holes are filled in. Thus, no tearing or gluing of the shape is permitted. The canonical example is that of a donut and a coffee cup. Since such a deformation exists by filling the cup and then inflating the handle, these daily objects occupy the same topological class.

In contrast, the distinction between a donut and an orange represents objects from distinct topological classes, as one would be required to poke a hole in the orange or tear the donut to construct a deformation. Such a deformation would not be continuous. Each geometric surface is a member of precisely one topological class, known as a genus; see Figure 1.1 for a helpful visualization of these classes. This notion of genus provides structure to the set over which the topological space is constructed, much like the way vector space or group axioms define the respective structure.
of the space. The relationship between these classes and the categorization of topological phases is profound and forms the basis for the current understanding of quantum materials. The notion of topological structure has contributed significantly to many fields of scientific research. From the topological classification of RNA [10] to knot theory of tori [11], applications of topology are widespread in modern scientific research. The motivation behind using topology as a tool in condensed matter physics is straightforward. Beginning in a microscopic scale, the field starts with a clear notion of spacetime as defined by the Minkowski metric. However, once the integer quantum Hall effect was discovered, the presence of spacetime distances dissolves, and the physical properties are governed by criteria which are robust against spacetime distance. The use of topology to describe the order in condensed matter systems proved invaluable in classifying these systems.

Band theory of solids

Before introducing the more intricate and multifaceted nature of topological electronic band structures, this section discusses the fundamentals of band theory in the context of relatively simple insulators, semiconductors, and conductors.

To lay the foundation of how bands occur in a crystalline sample, we will expand the notion of
smaller systems (concerning scale). Generally, electrons in isolated atoms live in atomic orbitals occupying discrete energy levels. If atoms are bonded, their orbitals join together, overlapping. However, due to the Pauli exclusion principle, multiple electrons cannot share the aforementioned discrete energy levels. As a result, each discrete energy level is split into differing, discrete energy levels. This process is known as hybridization. Suppose this process is repeated \( N \) times, as in a repeating crystal lattice; each atomic site overlaps with numerous others. Thus, the discrete energy values are split \( N \) times. In the case of a physical crystal sample, where \( N \approx 10^{22} \), these discrete values of energy are separated by such a small value that the states approach that of a continuous structure, known as a band [13, 14].

It should be noted that this process happens primarily with the outermost orbitals of each atom. Electrons occupying these orbitals are known as valence electrons and are associated with many chemical bonding properties and electrical conductivity. The outer bands that these electrons occupy are called valence bands, whereas the next outermost (higher in binding energy) bands are called conduction bands. How these bands touch or are gapped significantly influences a material’s transport properties. Insulating materials have large gaps, meaning electrons require a significant jump in energy to enter the conduction band. Semiconductors have small gaps, and conductors (metals) have little to no gap. Semimetals live somewhere in between these classifications. Often, the bottom of the conduction band is offset in momentum to the top of the valence band. This type of bandgap is known as an indirect bandgap.

Band theory in crystaline solids (materials which form solids in repeating, periodic lattices) is fundamentally influenced by Bloch’s theorem. Generally, the theorem states that the wave function of electrons in the crystal are restricted due to periodicity of the atomic sites. One may write it as:

\[
\psi(r) = e^{i\mathbf{k}\cdot\mathbf{r}}u(r).
\]  

\[ (1.1) \]
Where $\psi(r)$ is the wave function for an electron in the crystal, with $r$ is a space coordinate corresponding with the geometry of the crystal lattice, and thus $u(r)$ is some function of the space coordinate. Here, $k$ is the usual wave vector in reciprocal space according to:

$$\lambda = \frac{2\pi}{|k|}.$$  

(1.2)

To investigate the nature of electronic states, one must consider a particular vector (or set of vectors) for $k$. This allows computation of the energy eigenvalues to be computed, yielding information about the dispersion of electronic states along a direction in reciprocal space. The most common choices for $k$ as well as the simplest, are those along high-symmetry directions in the crystal. These directions give simple relations between components of $k$ like $k_x = k_y = k_z$ in the case of a cubic lattice. This strategy is further extended to non-cubic structures which are described in reciprocal space by relations such as $k_x = \sqrt{2}k_y$.

The next natural extension of this approach is to consider $k$ vectors according to parameters of the Brillouin zone. While not often as straightforward to obtain direct descriptions of energy bands, one may still obtain useful information like the density of states. [15]. Bands may or may not have ranges of energy where no electronic states may occur. These are called band gaps, and they play a major roll in how easily a material conducts. Conductors have no band gap, whence electrons can easily flow between conduction and valence bands. Semiconductors have small band gaps, where electrons require a small “boost” of energy to jump to the conduction band. This energy may come from thermal energy, in which case one may understand the decrease in conductivity of semiconducting materials as temperature decreases. Insulators have the largest band gaps; in this study, we will focus particularly on small band-gap insulators, semiconductors, and semimetals. Semimetals are characterized by a small, indirect, negative bandgap.
Quantum Hall and quantum spin Hall states

Stemming from the quantum Hall effect (QHE), the topological insulating state is easily seen by observing the cyclotron motion of electrons in the presence of a perpendicularly applied magnetic field. Electrons undergo circular motion according to the Lorentz equation:

$$F = qE + qv \times B$$  \hspace{1cm} (1.3)

See Figure 1.2 for a helpful schematic showing this process. Extending this notion towards an interface between two such materials gives the true notion of the quantum Hall state. As electrons undergo this circular motion, we note the unique behavior of electrons at the interface; they cannot complete each circular loop. Thus, they proceed along the interface as depicted in Figure 1.3(a). As a result of this chiral edge behavior occurring strictly at the surface, a single edge state then
connects the otherwise gapped valence and conduction bands in momentum space. This singular state thus now means there is an *odd* number of crossings of the Fermi energy $E_F$. Most importantly, these states travel in *one direction only*; this fact forms the basis for a significant portion of the potential applications of TMs to lossless electronics. Intrigued by the implications of the quantum Hall effect, the condensed matter community probed the possibility of if such a state could occur in the protection of time-reversal symmetry. Mele and Kane answered this very question by proposing the existence of such a state in graphene. Kane and Mele posited that graphene, an insulating and non-magnetic system, could host a new topological phase that arose from spin-orbit coupling (SOC) instead of magnetic fields [16]. Naming it the quantum spin Hall effect (QSHE), they proceeded to publish work on the $\mathbb{Z}_2$ topological invariant, which distinguished the QSHE from ordinary insulators [3]. Figure 1.4 shows a helpful visualization of the QSHE in an insulator like graphene. Note how the edge states corresponding to up and down spin travel in opposite directions. These states thus correspond to two spin-polarized bands in the band structure seen in Figure 1.4(b). Now that we have established the principles behind a TI, it is natural to extend this
thinking to consider other ways topologically protected states may present themselves. In the case of a TI, the introduction of magnetism may have a few notable effects. Firstly, chemical doping may be investigated. Chemical doping may shift electronic states based on the inclusion of p- or n-type dopants. If the dopant brings magnetism, then the doping process may be used to investigate the role magnetism plays in the topological phase. Doping has also allowed for observation of more exotic phenomena, such as the quantum anomalous Hall effect (QAHE)\cite{17, 18}. Secondly, doping TIs with transition metals typically induces a magnetic moment interacting with the topologically protected surface state. It is these two properties of many TIs that have drawn many to understand the nature of the relationship between topological states and magnetism \cite{19}. The process of magnetic doping is interesting as the introduction of magnetism breaks time-reversal (TR) symmetry. In combination with the considerations of doping listed above, breaking TR and/or inversion symmetry opens doors to more topological phases.

Lastly, it should be noted the importance of crystal structure in the study of TMs. Each material’s crystal structure, characterized mathematically as a “space group,” holds valuable information re-
garding the symmetry of repeating crystalline lattice. Numbered with natural numbers up to 230, each space group describes a unique combination of symmetries in the lattice’s structure. For example, Bi$_2$Se$_3$, one of the first investigated TIs, crystalizes with trigonal symmetry in a rhombohedral lattice, with space group number 166 [20]. Theorists have developed many criteria to narrow down the scope of materials being investigated experimentally. Often, this process involves considering the aforementioned symmetry (or asymmetry) of the band structure along axes of high symmetry within the system [21, 22]. This mapping of the unit cell in terms of energy-momentum dispersion defines the Brillouin zone (BZ), which is simply a unit cell in momentum space.

3-dimensional TI

Historically, the 3D topological insulator was first examined in the Bi$_{1-x}$Sb$_x$ system. This observation was new in that one could not reason these surface states in terms of the quantum spin Hall state. That is, linear momentum and spin of these electrons are “locked”, and thus the Berry phase is nontrivial at $\pi$ [4, 23, 24]. In the Bi-Sb system mentioned above, the small gaps decrease in size upon the introduction of Sb. The gap closes entirely at a concentration near $x \approx 4\%$, and a 3D Dirac point is present [25]. It was here that the 3D TI was first investigated, and it should be more apparent how new families of TMs are predicted, discovered, and explored.

Topological semimetals

We will explore the topological semimetals family by extending the notion of topological phases above. The most straightforward case can be realized first through a thought experiment. Recall that, for the TI we discussed above, a surface state forms that crosses the Fermi level at one point in the BZ, bridging valence and conduction bands along the surface. Topological semimetals (TSM)
instead host bulk band crossings. How these band crossings present themselves in tandem with crystalline and temporal symmetries provides the basis for classes of TSMs. First, we introduce the Dirac semimetal. By employing symmetry requirements of the eigenvalues in the $nth$ band of a solid, one may show how two crossing bands may interact and form a protected point, preserved by the enforcement of crystalline symmetry. This property, when applied to band inversion, is the principle behind the Dirac semimetal, depicted in Figure 1.5. The introduction of an applied magnetic field breaks time-reversal (TR) symmetry in the system. In this case, Dirac nodes split into two Weyl nodes, defining the Weyl semimetal.

The study of topological semimetals has grown significantly since their first discovery, with many classifications and families being predicted and experimentally realized. The nodal-line semimetals (NLSM), which will be investigated in this thesis, are characterized by a particularly unique band crossing. NLSMs present bulk band crossings which proceed along a line or closed loop in momentum space. [26]. TSMs are further divided into nonmagnetic and magnetic types based on breaking TR symmetry in magnetic systems. With the early discovery of the ZrSiS nodal-line family [27], there has been a significant push to uncover the properties of NLSMs [28–30]. The ZrSiS family, in particular, opened the door to investigate multiple related NSLSMs, as they hosted diamond-shaped fermi surfaces due to the Si square-nets[27]. The nodal-line state is fascinating due to its potential implications for superconductivity. Due to the flatness of surface states present in many NLSMs, exotic phenomena such as surface superconductivity may arise [31, 32]. A NLSM can be realized based on a Dirac-type or Weyl-type organization depending on the breaking of symmetries. With TR symmetry protected, a centrosymmetric material may host a Diract-type nodal line. This distinction requires weak spin-orbit coupling, where a strong SOC may gap out the nodal line, leading to a TI phase [33]. A helpful visualization of the nodal line and nodal loop can be seen in Figure 1.6. Finally, materials with non-symmorphic, glide mirror, or screw rotation symmetry may host NLSM phases, as the SOC is limited due to translation protection by the lattice
Figure 1.5: Schematic depicting the process by which an (a) uninverted band structure undergoes band inversion. (b) The twofold degenerate bands avoid a crossing by mixing parity (denoted +, -), maintaining a gapped state. However, mixing of parity may be forbidden along high-symmetry lines in the BZ, if enforced by crystalline symmetry. (c) Shows the resulting fourfold degenerate point, from [5].

symmetry [27, 34–36].

Selecting candidate materials

One issue arises when predicting which materials may host topologically nontrivial electronic states. With a seemingly endless number of materials with well-understood basic properties, one may find themselves overwhelmed. Here I will discuss a simple strategy for predicting a material’s topological classification. Because the first predictions of topological insulators largely influenced this process, I will present this process in that context. Insulators, in the general sense, are materials with what’s known as a “band gap,” which separates filled and empty energy bands. We may more precisely say that such materials exhibit local electronic phenomena. In this way, a simple insulator is “insensitive” to boundary conditions, where all electrons are localized to atoms. There is minimal sensitivity to external magnetic flux in a connected sample shaped into a ring, for example [37]. However, the mere existence of such an energy gap does not necessarily imply
robustness against boundary conditions. The simplest example is considering a system exhibiting the integer quantum Hall effect (IQHE). Multiple phases with bulk band gaps are all distinguished by differing topologies. The much celebrated Fu Kane criterion describes this distinction and can be an excellent predictor of a material’s topology [37].

To use this criterion in practice, a calculated band structure for a given material is typically used, the most well-known method being density functional theory (DFT). In particular, DFT proves helpful as the number of electrons in a given system increases, where computational power required in conventional quantum chemistry approximation grows exponentially compared to a 3rd power growth in DFT [38]. Once a material’s band structure is predicted with DFT, band crossings, band inversions, flat bands, and topological phases may be considered. Ultimately, the resulting 2D band structure is defined by a mapping from momentum space to the Bloch Hamiltonian. With the crystallographic momentum $k$ being defined on a torus, these gapped band structures are thus organized by the equivalence classes of the Hamiltonian. It is this notion that describes the foundational emphasis on topology in quantum materials [2].
Furthermore, topological materials are typically understood within the context of their other transport and magnetic properties, with the priming motivation being that they strongly influence any topological surface states which may be formed. Topological surface states may only arise in particular magnetic phases which transition at particular temperatures. In addition, some magnetic and transport markers are used as a flag which draws interest to particular families of compounds. Thus, by employing first-principles calculations in tandem with transport properties, one obtains a more holistic understanding of the origin of any topological phases.
CHAPTER 2: EXPERIMENTAL METHODS

Using high-quality angle-resolved photoemission spectroscopy (ARPES), this thesis will investigate a few compounds from multiple of the above families of topological materials. ARPES, which fundamentally relies on the photoelectric effect, provides insight into the occupation of electronic bands in a material. Put simply, an incoming light source with photon energy surpassing the material’s work function ejects electrons from the surface. The ejected electron travels through electronic lensing and a hemispherical analyzer. The hemispherical analyzer applies a known voltage across two hemispherical plates, which sort the incoming photoelectrons by kinetic energy $E_k$ and angle, thus in-plane momentum $k_{||}$. The emphasis here on the conservation of in-plane momentum by the electron is essential to a critical requirement in many ARPES labs: ultra-high vacuum (UHV). High pressures leave too many free gas particles between the surface and the analyzer. Hence, it becomes increasingly likely that photoelectrons collide with these gas particles, changing the electron’s momentum. ARPES is often performed at synchrotron light sources, providing photon energies in the ideal range for ARPES [39]. As seen in Figure 2.1, this is influenced by the mean free path of unscattered photoelectrons, which reaches a minimum at 20-100 eV [40]. This property characterizes ARPES as having extreme surface sensitivity at these photon energies. As a result, sample surfaces must be as atomically clean as possible. Any surface oxidation, impurities, or dust will drastically affect the collected data such that it diverges considerably from expectations.

Angle-resolved photoemission spectroscopy

To understand the physical requirements of ARPES data collection, we cover the main criteria and resulting states associated with photoemission, first.
Albert Einstein first pioneered the modern understanding of the photoelectric effect in a monumentally influential paper, focusing on quantized physical phenomena which diverge from classical counterparts [41]. The photoelectric effect is typically understood in the following manner: when incoming light interacts with an electron via the electromagnetic force, energy is transferred. If the photon has sufficient energy to remove the electron from the material, the electron may be ejected. For a surface electron, one may write the electrons kinetic energy after ejection as follows:

$$E_k = \hbar v - \Phi,$$  \hfill (2.1)

where $\phi$ is the work function, and typically lies near 4.5 eV for our purposes. To eject electrons which occupy higher binding-energy states, the incoming photon must have energy sufficient to overcome both the work function $\Phi$ as well as the binding energy $E_B$. In such a case, these ejected core level electrons would have kinetic energy

$$E_k = \hbar v - \Phi - |E_B|. $$  \hfill (2.2)

**Mean free path and probing depth**

Once excited, the electron travels to the sample surface. This process is not guaranteed, and the probability the electron reaches the surface is a function of its inelastic mean free path. This parameter represents the average distance the electron travels between inelastic collisions. So, the larger the mean free path of the excited electron, the deeper into the sample one is probing. In the study of quantum materials, we ideally aim to view electronic states as close to the surface as possible. Thus, the motivation behind photon energy choice is clear, as illustrated in Figure 2.1,
where inelastic mean free path is shown to reach a minimum in the range of 20-150eV. To consider contributions from the bulk electronic states, we may increase the probing depth by using lower photon energy light sources (like UV) or very high photon energy light sources like those available in synchrotrons.

Conservation equations

By conserving kinetic energy and components of momentum of a photoelectron, we may examine the state of the electron the instant before ejection. From above, we have the kinetic energy of a photoelectron, and thus the momentum in wave vector units:

\[ \mathbf{K} = \frac{1}{\hbar} \sqrt{2mE_k}, \quad (2.3) \]
Where $E_k$ is the kinetic energy as defined in equation 2.2. Writing as a vector according to the geometry definition in Figure 2, we may express the momentum as a sum of components parallel and perpendicular to the plane of the sample surface. Each component depends on the kinetic energy and angle of ejection,

$$K_{||} = \frac{1}{\hbar} \sqrt{2mE_k \sin(\theta)},$$

and similarly for the perpendicular component,

$$K_{\perp} = \frac{1}{\hbar} \sqrt{2mE_k \cos(\theta)}.$$  

(2.4)

(2.5)

Foundational to this rather elegant result is the assumption that the incident photon has negligible mass compared to the electron. With this assumption we have that, since the photon-electron interaction exchanges no momentum, the photoelectron has the same parallel momentum inside the crystal as outside. We denote the momentum inside the crystal as ($k_{||}$), giving:

$$k_{||} = K_{||}.$$  

(2.6)
This assumption is incredibly valuable as we need not keep track of the geometry of how the incident photon beam strikes the sample. If this were not the case, ejected electrons may have drastically different \( k_{||} \) to \( K_{||} \) depending on the angle of incident light.

Finally, defining the sample surface as the xy-plane, we may write \((k_{||})\) in terms of the x and y components within the crystal. Note that this vector is still in wave vector units, and hence lives in k-space (or reciprocal space). That is, the x and y directions refer not necessarily to values in \( \mathbb{R} \), but the notion is nonetheless similar. We simply define the azimuthal angle of the photoelectron as \( \phi \). Then, \( k_x \) and \( k_y \) can be written:

\[
k_x = \frac{1}{\hbar} \sqrt{\frac{2meE_k \sin(\theta) \cos(\phi)}}
\]

and

\[
k_y = \frac{1}{\hbar} \sqrt{2meE_k \sin(\theta) \sin(\phi)}.
\]

Finally, the value of \( k_z \) may be obtained after some assumptions regarding the dispersion of electrons in the final states of photoemission [39].

\[
k_z = k_\perp = \frac{1}{\hbar} \sqrt{2m(E_k \cos^2(\theta) + V_0)}
\]

In this case \( V_0 = |E_0| + \Phi \), is known as the inner potential, representing the energy at the bottom of the valence band with respect to vacuum. Thus, knowing \( E_k \) (which depends on \( h\nu \), \( \theta \), and \( V_0 \), gives a determined value of \( k_z \). So, \( k_z \) may be varied through the photon energy, which allows us to sweep through the Brillouin zone.
Physical experimental components

Included here is a brief discussion of the physical apparatuses involved in an ARPES lab as well as a general guide to sample preparation.

Geometry of the analyzer

The hemispherical analyzer functions on similar principles to a traditional mass spectrometer. An overview of its design elements and their implications are given here. A constant voltage is applied to two concentric hemispherical plates. In the radial direction, electrons are sorted by their kinetic energy. For two photoelectrons that are incident at the same angle $\alpha$ as seen in Figure 2.3, the electron which has larger kinetic energy (and thus velocity) will land radially outward compared to the other. It is in this way that the analyzer sorts electrons by kinetic energy. Similarly, travelling azimuthally along the analyzer represents differing angles of emission, or equivalently values of $k||$ as given.

Sample preparation

To ensure an atomically clean sample surface, samples must be cleaved under UHV conditions. Otherwise, thin layers of gas, oil, dust, or debris may land on the surface of the sample. Most laboratories employ a series of load-locks, garages, and other auxiliary chambers to make the loading process more efficient. Laboratory setups for ARPES often utilize different mounting mechanisms for samples, but they all tend to follow the same basic approach for examining single crystals. In this thesis, the following general approach was utilized, as depicted in figure 2.4.

1. First, samples are selected based on visual inspection. Sample size and apparent uniformity
are the primary criteria.

2. Next, a one-to-one mixture of A and B components of a silver epoxy is created. Sometimes, Torr Seal, a nonconducting adhesive is used. In these cases, graphite must be added to ground the sample and prevent charging.

3. A small dab of the mixture is placed onto the sample mounting plate, and the sample is gently placed on top.

4. The sample and mounting plate or post are left to cure on a hot plate for about 1 hour.

5. Steps (2) - (4) are repeated to mount a ceramic post on top of the sample. The post should be marginally smaller in diameter than the sample size.

The samples are now ready to be loaded. To load samples, the load lock is vented (typically with nitrogen) and exposed to atmospheric pressure. Then, the samples are carefully transferred into the load lock. The load lock is sealed, and the roughing pump (and then the turbo pump) is turned
on. Once the chamber has reached sufficiently low pressure, the samples may be transferred to additional load locks, garages, or the manipulator arm for analysis.
While not all the samples discussed here were grown in the lab, understanding basic growth methods is essential to the physical aspects of ARPES experimentation. Due to the aforementioned restrictions, samples must be loaded and cleaved under vacuum, either inside a load lock or the main chamber [39]. As a result, choosing high-quality samples that are more likely to cleave cleanly is essential to use beamtime efficiently. As a part of this project on quantum materials, we have begun setting up a crystal growth laboratory with our space in Research 1.

Growth methods

Modern applications of ARPES to study topological materials fundamentally rely on the ability to grow or acquire high-quality samples. Furthermore, bulk crystals may be thinned down towards a singular monolayer to investigate how the electronic states evolve as the system approaches the two-dimensional case. This section discusses some growth methods which are particularly simple and helpful for bulk single-crystal synthesis.

**Solid-state reaction**

A common and comparatively simple growth method is based on the solid-state reactions of crystal formation. It is this process that we’ve employed here. The process involves mixing high-purity elemental samples in their respective stoichiometric ratios. Then, the mixture is placed in a quartz ampule and evacuated (sometimes purged with inert gas). After being sealed, the ampule is placed in a furnace and heated above the melting temperature according to previous phase stability studies. Finally, the mixture is allowed to cool very slowly, often in the range of 3° C/hr. It is in this stage
that crystal domains are forming. Thus, it is imperative that this cooling occur slowly.

Flux method

Next, due to space considerations, I will briefly introduce another popular growth method used. Known as the “flux method,” a sample is grown as follows. First, the precise stoichiometric ratios of high-purity chemicals are powdered and mixed. A catalyst, referred to as the flux, is added to catalyze the crystallization process. With the flux added, the mixture is enclosed in a vacuum-sealed quartz ampule. By repeatedly pumping out the ampule and filling the chamber with inert gas, we aim to reduce the possibility of chemical reactions that could form oxides and impurities in the sample. After this process, the ampule is pumped down one final time and then sealed. Next, the sample mixture is left in a furnace that heats the ampule above the melting point (which is ideally lower now that we’ve added a catalyst) and very slowly cools the sample through the melting point. At this point, bonds within the sample form that result in grains of small, mostly uniform crystals suspended in a flux mixture. A centrifuge is typically used to remove the flux; applying a strong centrifugal force directly after removal from the furnace pulls out much of the flux from the mixture. Of course, a hurdle associated with the flux method is that completely removing the flux after crystal formation can prove difficult. A flux coating may ruin many otherwise high-quality samples. Removing this flux using acid baths can be possible, but I will omit this discussion here.

Characterization methods

One must consider the many possible crystallization phases for particular compounds. Simply mixing stoichiometric ratios is no guarantee that the desired phase will appear. Mixtures often coagulate and crystalize in multiple domains depending on thermodynamic conditions. Thus, any
sample growth project is best confirmed by chemical makeup and crystal structure measurements by utilizing energy-dispersive spectroscopy and X-ray diffraction, respectively [43].

\textit{X-ray diffraction}

X-ray diffraction (XRD) is a key technique in characterizing solid crystalline compounds. Results from XRD analysis give critical information about the sample’s crystal structure, phases, preferred orientations, and other useful crystal parameters. Also, the utility of XRD’s nondestructive nature should be noted, meaning it’s particularly useful in forensic science, geology, microelectronics, and many more industries. Now a standard practice in condensed matter physics, XRD is often set up as follows. X-rays are produced by a cathode ray tube and are subsequently filtered to produce monochromatic light. Monochromatic X-rays are then directed toward the sample, where the incident radiation interacts with the sample’s atomic sites, producing constructive or destructive interference. As a photon source, X-rays are particularly useful for this application as their wavelengths are comparable to the interatomic distance of crystalline solids. Electromagnetic radiation entering the material obeys Bragg’s condition:

\[ n\lambda = 2dsin\theta. \]  

(3.1)

Here, \( d \) is the atomic spacing responsible for diffraction, \( \theta \) is the angle of diffraction, \( \lambda \) is the wavelength of incident light, and \( n \) is an integer. Bragg’s condition specifies the conditions under which incoming electromagnetic radiation penetrates, diffracts, or is absorbed into the materials. Diffracted X-rays are then counted as the sample is scanned. Thus, particular angles which satisfy the Bragg condition according to the geometry of the diffractometer correspond to specific configurations of atoms within the crystalline lattice. By performing a scan through a range of \( 2\theta \), all possible diffraction patterns are obtained. [44] The obtained diffraction pattern can be used
as a fingerprint for each material, given the crystal structure and atomic lattice parameters which give the space between atoms. By comparing experimentally observed diffraction patterns with published results on known materials, a match may be found which may confirm lattice structure of the material.

*Energy-dispersive X-ray spectroscopy*

Energy-dispersive X-ray spectroscopy (EDS, EDX, or EDAX) is a similarly powerful tool in sample characterization. EDS used in tandem with XRD provides researchers with two particularly key parameters in condensed matter research: crystal structure and chemical makeup. With XRD employed to characterize a sample’s crystal structure, a sample’s chemical makeup may still be ambiguous. That is, there may be unknown dopants or impurities which still crystalize in the same structure as a parent material. Thus, to examine the specific stoichiometric ratios of present elements, we examine the sample using EDS.

EDS fundamentally relies on the emission of characteristic X-rays. As electrons transition between inner orbitals, they release electromagnetic radiation as a function of the energy difference between their initial state $E_i$ and final state $E_f$: $\Delta E = E_f - E_i$. See Figure 3.1 for a helpful visualization of this process. X-ray energies for these purposes mostly range between 1-10KeV and correspond to a particular set of orbital transitions. Electrons must be first “knocked out” of their inner orbitals to induce photon emissions of this energy. Once an electron is ejected, another from a higher energy level fills its vacancy. These electron vacancies in energy levels are produced by an external bombardment of electrons or X-rays. An X-ray spectrometer (enabling EDS) is often added to an existing scanning electron microscope (SEM). Thus, the electron beam used for SEM is a common source for EDS. X-ray lines are identified using a combination of Roman and Greek letters and numbers. The Roman Letter (K, L, M) indicates the energy shell or quantum number, and a
Figure 3.1: Schematic showing the electron de-excitation transitions for Iodine, from [45].

Greek Letter ($\alpha$, $\beta$, etc.) is used to indicate the group that the line belongs in order of decreasing importance. Finally, a number denotes the decreasing line intensity within the group (1, 2, etc.). For example, the most intense lines are $K\alpha_1$, $L\alpha_1$, and $M\alpha_1$. Some lines may have low enough intensity or correspond to an energy transition close enough to another to be undiscernible. For example, the $K\alpha_2$ line is often unresolved, so the corresponding peak may be designated $K\alpha$ or $K\alpha_{1,2}$.

Materials grown: Bi$_2$Se$_3$

As an ongoing project to expand our group’s versatility, this section is focused on elucidating the progress made in developing a crystal synthesis lab in our auxiliary space in Research 1.
**Crystal synthesis**

Stoichiometric ratios of Bismuth (Bi) and Selenium (Se) were measured according to their 2:3 molar ratio in Bi₂Se₃. After being powdered and mixed in a mortar and pestle, the contents were transferred to two quartz tubes. In one ampule, the sample was first placed into ceramic crucibles and compacted with quartz wool. Both ampules underwent the following process. First, a small neck is created on the open end of the ampule. This neck will be used for pumping and venting with argon. Insulating the sample from the oxygen torch used to work the quartz is essential. If not, the sample may undergo some reactions with oxygen in the tube. This process was accomplished by wrapping the bottom half of the ampule in a wet paper towel. Next, the ampule is connected to a T splitter, which may be connected to an Argon gas supply or a vacuum pump. The ampule is repeatedly pumped and vented with argon. Pumping and venting remove as much oxygen and potential reactants from the ampule, so minimal chemical reactions occur in the furnace (besides crystal formation). Finally, after multiple iterations, the neck of the ampule is once more heated and sealed off. The ampule is then let to cool briefly before being transferred to the furnace. In the furnace, the ampules (one with crucibles and one without) are set to follow a pre-programmed multi-stage heating process. Following the general procedure outlined by the solid-state growth discussion above, the furnace was programmed according to the heating profile shown in Figure 3.2. Once the furnace is cooled, the ampules may be removed and carefully broken open to reveal resulting samples.

**Sample characterization**

Multiple resulting crystals appeared to be of high quality. Figure 3.3 shows photos taken of some of these samples under an optical microscope. The grid lines in (b) are spaced every 1mm, for scale. Crystals ranged in size from 1 mm to 15 mm. Some flat and shiny domains can be seen,
Figure 3.2: Heating profile used for sample growth of Bi$_2$Se$_3$.

Figure 3.3: Sample photos taken using an optical microscope.
which may indicate relatively uniform and atomically flat surfaces. To confirm the quality, a few of the best samples were characterized further. Next, some samples were chosen for XRD analysis to examine crystal structure and the growth methods’ effectiveness. Performing XRD on a high-quality Bi$_2$Se$_3$ single crystal yielded a convincing diffraction pattern that closely matched other reported XRD results. The results are shown in Figure 3.4(a). Data was collected on XRD #1 at
the Materials Characterization Facility (MCF) in the Advanced Materials Processing and Analysis Center (AMPAC) at the University of Central Florida. XRD #1 is a PANalytical Empyrean with a 1.8 kW Copper (Cu) X-ray tube, utilizing a Kα filter for these measurements. We see clearly defined and sharp Bragg peaks due to the (001) orientation. Since the bismuth-selenide system has become commercially popular, we may also consider standardized XRD measurements performed on (001) Bi$_2$Se$_3$ single crystals. Also, confirming the results with peer-reviewed journals gives confidence that the grown sample was of the intended crystal structure [47, 48].
CHAPTER 4: ARPES MEASUREMENTS OF A RARE-EARTH-BASED SEMIMETAL

The results presented in this chapter have recently been accepted for publication in Physical Review Materials. A pre-print is available at [49].

Introduction

Lanthanide (Ln)-based LnSbTe systems represent relatives to the ZrSiS family, and have gained prominent attention recently for introducing magnetic moments to previously studied nonmagnetic materials like ZrSiS. Through the choice of Ln element comes the ability to observe the evolution of the electronic structure, providing insight into the relationships between topology, magnetism, and electron correlation. The antiferromagnet GdSbTe hosted a nodal-line state in addition to an antiferromagnetic Dirac state, with a Néel temperature of 12K [50, 51]. CeSbTe has also been predicted to potentially host topological states [52]; HoSbTe [53], LaSbTe [54], and SmSbTe [55] have all also been investigated and either shown or predicted to host topological surface states. By comparing the electronic structure of NdSbTe to the rest of the family, along with the relevant magnetic and transport properties [56], this study aims to aid in the understanding of how the choice of Ln element affects the electronic structure. With the Nd-based member of this family remaining unstudied in terms of experimentally observed electronic structure, this project aims to add a piece to the puzzle that is nodal-line semimetals in the LnSbTe family. Transport and magnetic measurements of NdSbTe have been performed and published [57, 58]. However, without experimental measurements, the full picture of this system has yet to be elucidated. In this chapter, an in-depth study of the NdSbTe system is presented via ARPES, thermodynamic measurements, and first-principles calculations.
(a) Crystal structure in three dimensions.

(b) Transport measurements.

Figure 4.1: Crystal structure and bulk transport and magnetic measurements. (a) Crystal structure shown in three dimensions with a, b, and c vectors labelled. Teal, magenta, and blue spheres represent Nd, Sb, and Te atoms, respectively. (b) Measured temperature dependence of specific heat, with an included inset to show the low-temperature region. (c) Magnetic susceptibility dependence of temperature, with an applied field of 0.5 T parallel to the c-axis. The top left inset presents low-temperature region. Bottom right inset shows magnetization due to applied magnetic field at a fixed temperature of 1.72 K. A dashed line is included as a reference to see the resemblance to a linear trend.

Experimental and computational details

NdSbTe single crystals were grown using chemical vapor transport and subsequently characterized by EDXS and XRD. Heat capacity, magnetic susceptibility, and magnetization measurements were performed in collaboration using commercial units. The ARPES data shown here was collected at the Stanford synchrotron radiation lightsource (SSRL) endstation 5-2 at a temperature of 18 K. The lensing and aperture settings on the analyzer were set such that energy resolution was at worst 20 meV. DFT calculations were done using Vienna ab initio simulations using projector augmented wave potential [59–64].
NdSbTe crystallizes in a tetragonal structure, characterized by group $P4/nmm$, number 129. Nd-Te layers separate square Sb nets, shown in Figure 4.1. The thermodynamic measurements presented in (b) and (c) of Figure 4.1 help characterize the bulk transport and magnetic properties of the sample. High-temperature specific heat approaches 74 J/mol-K, remarkably close to the Dulong-Petit limit of 74.8 J/mol-K. A notable peak can be seen near the Neel temperature $T_N = 2.7$ K. To classify magnetic properties, the magnetic susceptibility is investigated. Another peak in magnetic susceptibility is seen near the aforementioned Neel temperature, which likely points to long-range antiferromagnetic ordering. The mostly linear nature of the magnetization dependence of applied field at 1.72 K (below $T_N$) shows antiferromagnetic behaviour, particularly below an applied field of 2 T, at which point a metamagnetic transition is seen. Previous electronic and magnetic studies reveal findings similar to those presented here [57, 58].
**Bulk band calculation**

Band structure calculations using DFT are shown in Figure 4.2. Finalized lattice structure parameters used were $a = b = 4.371$ Å and $c = 9.457$ Å. Previous values as reported in [66] are in close agreement. Figure 4.2(a) shows the 3D bulk BZ. The bulk band structure presented in (b) shows nodal lines along the X-R direction, boxed in green and red; these are due to the underlying symmetry group $P4/nmm$. Multiple linear Dirac crossings are shown near the X and R points, associated with the aforementioned nodal lines. Note also that the structure along the $\Gamma - M$ direction appears gapped in both cases.

**Fermi surface and constant energy contours**

As is often the case with materials in this family, the FS shows overall diamond-like pockets with $\Gamma$ centered in each diamond. Along the edge of the pocket shows two sheets, which converge upon decreasing binding energy about 300 meV below $E_f$. Another central pocket appears upon further decreasing of binding energy, eventually developing into a distinct diamond shape. Figure 4.3 shows the observed FS using 70 eV photon energy, where each of the two outer diamond-shaped sheets are faintly seen, with the inner pocket appearing and growing in size down to 650 meV below $E_f$.

**Gapless nodal lines**

The experimental realization of nodal lines in this material is presented here. The first nodal lines shown trace below the diamond shape of the FS. Figure 4.4 shows the horizontal and vertical dependence of the band structure along the $\overline{M} - \Gamma - \overline{M}$ direction. In the LV and LH polarizations, a singular, steep band is seen crossing the Fermi level slanting outwards and inwards, respectively. By adding the matrices of each polarization, we may construct a more representative experimental
Figure 4.3: Experimentally observed Fermi surface and constant energy contours. (a) FS measured using a 70eV photon energy, with horizontal polarization. (b)-(d) Experimental constant energy contours 300meV, 450meV, and 650meV below the FS. Equivalently, \( E - E_f = -0.3\text{eV}, -0.45\text{eV}, -0.65\text{eV} \).

distribution along this cut. As a result, we observe a linear crossing about 300 meV below the Fermi level. This crossing proceeds along the diamond shape seen, and thus explains the duality of the diamond sheets of the FS. We also present observation of the surface state at the \( \bar{X} \) point in Figure 4.5, shown along the \( \bar{M} - \bar{X} - \bar{M} \) direction. Using LH polarized light, we observe a gapped, Dirac-like state at \( \bar{X} \). This state has limited dependence on varied photon energy, and thus likely of surface nature. The robustness of this state as photon energy is varied is seen clearly in 4.5(a)-(c). The calculated dispersion along the same direction is shown in (d), where the gapped nature and overall shape agrees with experimental data. Next, we present the observation of the gapless nodal-line states, particularly along the \( \bar{X} - \bar{\Gamma} - \bar{X} \) direction. Most easily seen at 70 eV (\( k_z \approx \pi \)) photon
energy, a linearly-dispersive band is seen crossing the Fermi level at the $X$ point, clear in Figure 4.6(b). This band crossing moves down slightly as $k_z$ approaches 0 (at $h\nu = 60$ eV), and thus corresponds to the nodal line boxed in green from Figure 4.1(b). Another linear band crossing is seen at the $X$ point, about 750 meV below the Fermi level. This feature moves very little with photon energy, and thus corresponds to the nodal line along $X - R$ direction, boxed in green in Figure 4.2(b). The observed band structures are well supported by the calculated electronic band structure shown in Figure 4.6(d).
Conclusion

In conclusion, we conducted an in-depth study of NdSbTe’s electronic structure. Supported by ARPES measurements and first-principles calculations, we observe a diamond-shaped Fermi surface. The expected surface state occurring at the $\bar{X}$ point, due to the Sb square-net, was observed. Without the consideration of SOC, multiple nodal lines are predicted according to calculations. Some of these nodal lines gap out under the inclusion of SOC, particularly along the $X - R$ direction. Thus, we experimentally observe linearly-dispersive bands near the Fermi level along this
direction. Furthermore, we observe a nodal line along the $\Gamma - M$ direction which is sensitive to light polarization. This study contributes to the evolution of experimental realization of electronic structures in the $LnSbTe$ family.
CHAPTER 5: OUTLOOK & CONCLUSION

To conclude, multiple Bi$_2$Se$_3$ samples were grown using the Bridgman method. Optical microscope photos of the samples reveal some atomically clean surfaces. Preliminary XRD characterization shows discrete Bragg peaks that correspond with expected results for a single crystal oriented along (001). Next, NdSbTe, a member of the LnSbTe family, is investigated. By employing high quality ARPES, magnetic and transport measurements, and calculated band structures, we present multiple gapless nodal-lines. One circling the $\Gamma$ point, as well as two along the $X – R$ direction. Theoretical calculations predict the former to be gapped, but experimental results show gapless structure within the 20 meV energy resolution of the analyzer. These results add insight into the progression of the aforementioned rare-earth based family of materials and the potential applications of these materials to electronics.
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