

Optical Investigation of Tungsten Diphosphide (WP_2), A Weyl Semimetal

by

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Declaration

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Approval

This dissertation of Nyirongo Racheal is approved as a partial fulfilment of the requirements for the award of the Degree of Master of Science in Physics, of the University of Zambia.

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Signature:

Supervisor:Date:

Signature:

Dedication

To my lovely mother,

This work is dedicated to you, for your unwavering love, support, and encouragement have been the foundation of my journey. Your sacrifices, wisdom, and strength have inspired me every step of the way. Without your belief in me, this achievement would not have been possible. This dissertation is not just my achievement, it is ours.

With all my love and gratitude, this is for you.

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Abstract

The optical investigation of tungsten diphosphide (WP_2), a type-II Weyl semimetal, reveals its exceptional topological and anisotropic electronic properties. Through resistivity and Fourier-transform infrared spectroscopy measurements, WP_2 exhibit high conductivity and anisotropic transport behavior. Key findings include a high residual resistivity ratio (RRR) of 47,000, indicative of exceptional crystal purity and long electron mean free paths. At low temperatures, WP_2 exhibits quadratic temperature-dependent resistivity, aligning with Fermi liquid theory and underscoring the minimal impurity scattering in clean samples. The optical reflectivity and conductivity of WP_2 were obtained using Fourier-transform infrared spectroscopy, followed by Kramers-Kronig analysis respectively. WP_2 shows strong anisotropy between its a-axis and c-axis orientations, as evidenced by differences in plasma edges i.e. 3750 cm^{-1} for E//c axis plane and 3600 cm^{-1} for E// a plane axis and in the scattering rate. Anisotropy occurs when the refractive index of a material varies with polarization or propagation direction, enabling controlled modulation of light, which can be applicable in optical switching. The study also identified distinct interband transitions and directional variations in optical responses, with enhanced carrier mobility along the a-axis compared to the c-axis. Spectral weight analysis highlights a redistribution across the mid-infrared and near-infrared regions, consistent with WP_2 's robust electronic structure. These results establish WP_2 as a benchmark material for topological physics and a promising candidate for electronic and optoelectronic applications e.g optical switch.

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List of Abbreviations

TI	Topological Insulator.
WSM	Weyl Semimetal.
WP₂	Tungsten diphosphide (a Type-II Weyl Semimetal).
MR	Magnetoresistance.
FIR	Far-Infrared.
MIR	Mid-Infrared.
NIR	Near-Infrared.
NIR-VIS	Near-Infrared to Visible Range.
FFFIR	Far-Far-Far Infrared.
FFIR	Far-Far Infrared.
XRD	X-ray Diffraction.
XRO	X-ray Optics.
FTIR	Fourier-Transform Infrared.
MCT	Mercury Cadmium Telluride (detector).
SOC	Spin-Orbit Coupling.
BZ	Brillouin Zone.
RRR	Residual Resistivity Ratio.
E // a	Electric Field Parallel to the a - axis plane.
E // c	Electric Field Parallel to the c - axis plane.
DC	Direct Current.
ω_p	Plasma Frequency.
PID	Proportional-Integral-Derivative (controller)
ARPES	Angle-Resolved Photoemission Spectroscopy
WO₃	Tungsten Trioxide.
I₂	Iodine.
KBr	Potassium Bromide
CaF/ CaF₂	Calcium Fluoride.
Bi₂Se₃	Bismuth Selenide.

Na₃Bi	Sodium Bismuthide.
Cd₃As₂	Cadmium Arsenide.
TaAs	Tantalum Arsenide.
NbAs	Niobium Arsenide.
NbP	Niobium Phosphide.
WTe₂	Tungsten Ditelluride.
MoTe₂	Molybdenum Ditelluride.
HgTe	Mercury Telluride.
HeNe	Helium Neon

Chapter 1

INTRODUCTION

Topological materials are a new class of quantum materials in the field of condensed matter physics and materials science which were earlier predicated by theoretical physicists such as Charles Kane, Eugene Mele, Shoucheng Zhang and Colleagues in the 2000s [1]. The theoretical prediction were later accompanied by experimental discoveries of Topological Insulators (TI) such as Bismuth antimony alloys and Mercury Telluride [2]. The last decade has also seen the discoveries of a new class of topological materials; the topological semimetals, such as Dirac and Weyl semimetals which exhibit unique topological properties in their electronic band structures [3]. These properties are a result of underlying symmetry inversion or time-reversal symmetry which give rise to formation of exotic electronic states on the surface of the material. The discovery of such topological materials has led to the emergence of new phenomena of both topological insulators and topological semimetals which has the potential to revolutionize various technological applications [4].

Topological insulators and topological semimetals are both characterized by surface states induced by topology of the bulk band structure. The topological Dirac semimetal is a three-dimensional counterpart to graphene, which has been discovered to exist in Na_3Bi and Cd_3As_3 [5-8]. The gapless nature of the bulk band of Dirac semimetals brings rich physics into both the two and three dimensional electron gases. A Weyl semimetal (WSM) is a topological semimetal whose solid state crystal has low energy excitations known as Weyl fermions, which carry electrical charge at room temperature [9-10]. The study of these Weyl semimetals is therefore strongly driven by the search for the long sought after Weyl fermions. In 1929, H. Weyl found that a massless Dirac fermion could be decomposed into a pair of relativistic particles with opposite chirality; the Weyl fermion [11-14]. The Weyl fermion is a massless particle with half-integer spin that was once mistakenly thought to describe neutrinos, although not yet observed among elementary particles in high energy physics.

The bulk band structure in a Weyl semimetal features pairs of singly degenerate Weyl cones of opposite chirality and linearly dispersing valence and conduction bands in three dimensional (3D) momentum space that meet at discrete “Weyl points”. These Weyl points act as monopoles in momentum space with a fixed chirality that behaves as a source (“+” chirality) or a sink (“-” chirality) and they always appear in pairs. Chirality is a geometric property of a structure or object, meaning it cannot be superimposed onto its mirror image.

The breakthrough in the search for Weyl semimetals emerged from the TaAs class of materials [15-18]. Angle resolved photoemission spectroscopy (ARPES) measurements have explicitly proved that TaAs [19-22], NbAs [23, 24], TaP [25, 26], and NbP [27-30] are Weyl semimetals by direct observation of the linear dispersion of bulk Weyl cones and the arc-shaped surface states that terminate at the projected Weyl points on the surface. The four members i.e. (TaAs, NbAs, TaP and NbP) of this family share the same space group $I4_1$ md and a similar electronic band structure which features 12 pairs of Weyl nodes in the bulk bands and multiple Fermi arcs on the surface. Several key chiral Weyl fermion-induced phenomena have also been observed in electronic transport and optical measurements, such as the extremely large magnetoresistance [31], the helicity-protected ultrahigh mobility [32], the violation of Ohms law [33], the magnetic tunneling-induced Weyl node annihilation [34], the giant anisotropic nonlinear optical response [35], and the optical detection of Weyl fermion chirality [36] have been experimentally discovered. Among these experiments, two exceptionally remarkable achievements lie in the detection of the signature of the chiral anomaly effect [30, 37] and the axial-gravitational anomaly effect [38], which may open a new era of table-top experimental realizations of high-energy physics. Furthermore, the unusual spin texture of the Fermi arc surface state on TaAs has also been detected which has formed a basis for Weyl semimetals [30,39].

In WSMs the degeneracy is lifted owing to the breaking of the Inversion symmetry or Time-reversal symmetry or both. Theory predicted that these WSMs can be classified into type-I (e.g. TaAs, TaP, NbAs, and NbP) which respects Lorentz symmetry, and type-II (e.g. MoTe₂, WTe₂, and WP₂) which does not. Type-II Weyl fermions can further be viewed as tilted cone shaped dispersion in momentum space which breaks Lorentz symmetry and thus cannot exist as fundamental particles in nature. This type of Weyl fermion exists as a unique phenomenon of condensed matter physics. Distinct from type-II Weyl semimetals, type-I Weyl semimetal, from a material science perspective, can be treated as a direct negative band gap semiconductor while type-II Weyl semimetal features an indirect negative band gap. As one might expect, many more type-II Weyl semimetals than type-I exist in

real materials. Experiments have verified the existence of several new theoretically predicted Weyl semimetals including LaAlGe [40], TaIrTe₄ [41-43], Ta₃S₂ [44, 45], WP₂ class [46, 47], Mn₃Sn class [48-49], and β -Ag₂Se [50], which largely belong to the type-II Weyl semimetal category. Research into Weyl semimetals both in the context of new materials and new phenomena is, at present, an extremely dynamic field. Thus this dissertation focuses on the three dimensional transition metal diphosphide WP₂, which was recently predicted to host four pairs of type-II WPs (Weyl points) below the Fermi energy [51]. One important characteristic feature of this WSM (WP₂) is that the nearest WPs are of the same chirality and, therefore, it is robust against structural distortions or defects. One might then expect high conductivities which indeed were discovered in the studies of similar Weyl semimetals [52]. It is therefore, the Weyl fermions in the bulk and the Fermi arcs on the surfaces of Weyl semimetals that are of interest in condensed matter physics and material technology because their high mobility charged Weyl fermion find use in electronics and computing [53].

A few WSMs such as TaAs and NbP class have been used to demonstrate some properties of WSMs such as Chiral anomaly [30], Hall effect anomaly [27], Magnetoresistance (MR) and electrical transportation [36], but there is scant information about the optical properties of these materials. Hence, the aim of this dissertation is to explore the optical properties of WP₂, a type II Weyl semimetal and elucidate the underlying mechanisms governing its behavior through measuring its reflectivity and determining its conductivity through Krammers-Kronig analysis. To achieve this aim, single crystals of WP₂ were first characterized by X-ray diffraction (XRD), followed by resistivity measurements using the standard four-probe method. Finally reflectivity measurements were done using the Fourier-transform infrared spectrometer (Bruker Vertex 80v). From these measurements, optical conductivities have been obtained through Kramers-Kronig analysis. And from the optical conductivity other parameters like the mass enhancement factor, scattering rate and spectral weight have been obtained.

The current dissertation is organized as follows: First the optical properties of solids are reviewed, then an introduction to topological materials, a general overview of Weyl semimetals, a distinction between type I and II Weyl semimetals and tungsten diphosphide, (WP₂) in Chapter 2. This is followed by brief experimental descriptions of optical spectroscopy techniques and the analysis of optical data in Chapter 3 and 4, respectively. The results and discussions for single crystals of WP₂ sample are presented in Chapters 5, and finally a conclusion in chapter 6, respectively.

1.1 Aim/Purpose of The Study

To investigate the optical properties of the Weyl semimetal tungsten diphosphide (WP_2) single crystals using infrared spectroscopy.

1.2 Specific Objectives

- To measure the reflectivity of tungsten diphosphide (WP_2) single crystals.
- To determine the conductivity of tungsten diphosphide (WP_2) single crystals through Krammers-Kronig analysis method.

1.3 Research Question

How does the optical response of (WP_2) obtained in the study compare with those of other topological Weyl semimetals already known?

1.4 Significance of The Study

The knowledge obtained from the optical properties of the Weyl semimetal tungsten diphosphide (WP_2), in this study will add to the wealth of knowledge in the field of Condensed Matter Physics. Which will enhance its applications in spintronics, quantum computing, high-performance electronics, optoelectronics, thermoelectrics, and superconductivity.

Chapter 2

THEORETICAL BACKGROUND AND LITERATURE REVIEW

2.1 OPTICAL PROPERTIES OF SOLIDS

A metal is a solid held together by metallic bonds, conducts heat and electricity, reflects light, and whose resistivity usually decreases with decreasing temperature. Metals are materials with partially filled electron bands. Optical transitions between electron states in these partially filled bands (intraband transitions) together with transitions between different bands (interband transitions) are responsible for electrodynamics in metals [54]. The physical properties of metals are important in the understanding of Weyl semimetals. Further, the basics of electrons in solids and energy bands have to be known. Frequency dependent optical properties of metals can be described by the phenomenological Drude Lorentz and Sommerfeld models. The Drude Lorentz model is based on classical dispersion theory and is used to describe optical properties and the overall electrodynamic response of metals [54]. In this approach, the complex (optical) conductivity is then described by the sum of the Drude component and an appropriate number of Lorentz harmonic oscillators for the finite energy excitations. In sections which follow, brief descriptions of these models which are used to describe the optical properties of solids as presented in the dissertation of G. Chanda is hereby reproduced in section 2.1.1 and 2.1.3. [55]

2.1.1 Drude-Sommerfeld Model

The Drude model (1900) [56] regards a metal as a classical gas of electrons, which execute diffusive motion. In this model, electrons move freely in the lattice and there is no inter-

action between them. After an average time τ the electrons scatter completely inelastically with the lattice. The scattering rate ($\frac{1}{\tau}$) and the mass (m) of the electrons are independent of the velocity (energy). The existence of an average relaxation time τ which governs the relaxation of the system to equilibrium is the central assumption of the model. In the Drude model, the equation of motion for an electron in the presence of an applied electric field is given by:

$$m \frac{d^2 r}{dt^2} + m \frac{v}{\tau} = -eE \quad (2.1)$$

where $\frac{dr}{dt} = v$ is the velocity (v) and the current density is given by $j = nev$, with n being the density of charge carriers, m being the charge carrier mass, and e being the electronic charge. For dc fields, the condition,

$$\frac{md^2r}{dt^2} = 0 \quad (2.2)$$

leads to the dc conductivity, i.e.:

$$\sigma_{dc} = \frac{j}{E} = \frac{ne^2\tau}{m} \quad (2.3)$$

Upon the application of an alternating electric field of the form;

$$E(t) = E_0 e^{-i\omega t} \quad (2.4)$$

the solution of Eq. (2.1) becomes:

$$\sigma(\omega) = \frac{j}{E} = \frac{ne^2\tau}{m} \frac{1}{1 - i\omega\tau} = \frac{ne^2\tau}{m} \frac{1 + i\omega\tau}{1 + \omega^2\tau^2} = \sigma_1(\omega) + i\sigma_2(\omega) \quad (2.5)$$

With σ_1 and σ_2 and being the real and imaginary part of the complex conductivity, respectively. The average distance traveled by the electrons between collisions is called mean free path (l), and within the framework of the Drude model $l = \langle v \rangle_{th} \tau$, with $\langle v \rangle_{th}$ being the average thermal velocity. However, since electrons are fermions and as a result obey Fermi statistics, the picture is fundamentally different and the consequences of this were developed

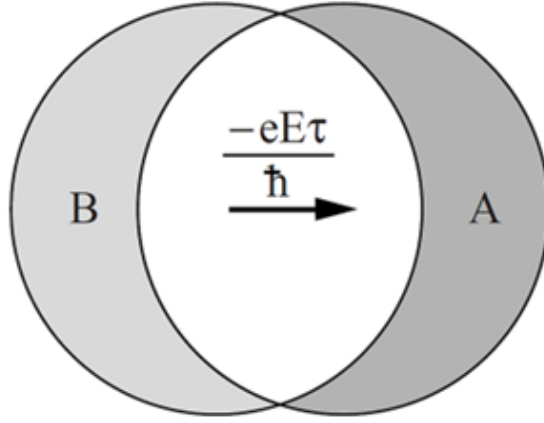


Figure 2.1: Displaced Fermi sphere in the presence of an applied electric field E . Electrons are removed from region B by the momentum ($p = -eE\tau$) and are added to region A. This figure applies to a metal with a spherical Fermi surface of radius kF or a circular Fermi surface in two dimensions. Picture taken from Ref [54]

by Sommerfeld [57]. Within Sommerfeld model, the concept of the Fermi surface plays a significant role. In the absence of the electric field, the Fermi sphere is centered around zero momentum while in the presence of the field E , the Fermi sphere is displaced by $\frac{-eE\tau}{\hbar}$. By this displacement, electrons are removed from one region (e.g. region B) and added to another region (e.g. region A) as demonstrated in Fig. 2.1. The equation of motion is the same as in the Drude model with $j = \frac{ne\hbar\langle k \rangle}{m}$. Where $k = \frac{p}{\hbar}$ (p being the momentum), and Eq. (2.5) is recovered. However, the scattering process which establishes equilibrium in the presence of an electric field involves only electrons near the Fermi surface and consequently, the mean free path $l = vF\tau$ (vF being the Fermi velocity) differs drastically from the mean free path given by the original Drude model and this difference has important consequences for temperature dependencies. The sum rules are valid, for example the sum rule for the real part of the optical (complex) conductivity is given by:

$$\int_0^\infty \sigma_1(w) = \frac{ne^2}{m} \int_0^\infty \frac{r dw}{1 + w^2 \tau^2} = \int_0^\infty \frac{w_p^2}{4\pi} \frac{d(\tau w)}{1 + (w\tau)^2} = \frac{w_p^2}{8} \quad (2.6)$$

With w_p being the plasma frequency and m the electronic mass. For a spherical Fermi surface,

$$w_p^2 = \frac{4\pi n e^2}{m} \quad (2.7)$$

Various optical parameters can be evaluated in a straight forward manner by just taking advantage of the optical conductivity as obtained by the Drude Sommerfeld model. Table 2.1 shows the relation between the material parameters and the optical constants (the dielectric constant ($\hat{\epsilon}$), the complex conductivity ($\hat{\sigma}$) and the complex refractive index ($\hat{N}$)). From Eq. (2.5), the dc limit of conductivity can be written as:

Table 2.1: Relationship between the material properties and optical constants [54].

	Dielectric constant $\hat{\epsilon}$	Conductivity $\hat{\sigma}$	Refractive index $\hat{N}$
$\hat{\epsilon}$	$\hat{\epsilon} = \epsilon_1 + i\epsilon_2$	$\epsilon_1 = 1 - \frac{4\pi\sigma_2}{w}$ $\epsilon_2 = \frac{4\pi\sigma_1}{w}$	$\epsilon_1 = \frac{n^2 - k^2}{\mu_1}$ $\epsilon_2 = \frac{2nk}{\mu_1}$
$\hat{\sigma}$	$\sigma_1 = \frac{w\epsilon_2}{4\pi}$ $\sigma_2 = (1 - \epsilon_1) \frac{w}{4\pi}$	$\hat{\sigma} = \sigma_1 + i\sigma_2$	$\sigma_1 = \frac{nk w}{2\pi\mu_1}$ $\sigma_2 = (1 - \frac{n^2 - k^2}{\mu_1}) \frac{w}{4\pi}$
$\hat{N}$	$n = \left\{ \frac{\mu_1}{2} [\epsilon_1^2 + \epsilon_2^2]^{1/2} + \frac{\epsilon_1 \mu_1}{2} \right\}^{1/2}$ $k = \left\{ \frac{\mu_1}{2} [\epsilon_1^2 + \epsilon_2^2]^{1/2} - \frac{\epsilon_1 \mu_1}{2} \right\}^{1/2}$	$n = \left\{ \frac{\mu_1}{2} \left[\left(1 - \frac{4\pi\sigma_2}{w}\right)^2 + \left(\frac{4\pi\sigma_1}{w}\right)^2 \right]^{1/2} + \frac{\mu_1}{2} - \frac{2\pi\mu_1\sigma_2}{w} \right\}^{1/2}$ $k = \left\{ \frac{\mu_1}{2} \left[\left(1 - \frac{4\pi\sigma_2}{w}\right)^2 + \left(\frac{4\pi\sigma_1}{w}\right)^2 \right]^{1/2} - \frac{\mu_1}{2} + \frac{2\pi\mu_1\sigma_2}{w} \right\}^{1/2}$	$\hat{N} = n + ik$

$$\sigma_1(w=0) = \sigma_{dc} = \frac{ne^2\tau}{m} = \frac{1}{4\pi} w_p^2 \tau = ne\mu \quad (2.8)$$

where $\mu = \frac{e\tau}{m}$ is the electron mobility; while, $\sigma_2(w=0) = 0$. For $w \rightarrow \infty$, $\sigma_1(w) \propto \frac{1}{w^2}$ and $\sigma_2(w) \propto \frac{1}{w}$. By using the relationship between σ and ϵ in table 2.1 we have, $\epsilon_1 = 1 - 4\pi\sigma_{dc}$ and $\epsilon_2 = \frac{4\pi}{w}\sigma_{dc}$ for $w \rightarrow 0$ while for $w \rightarrow \infty$, $\epsilon_1 = 1 - \frac{4\pi}{w^2\tau}\sigma_{dc} \propto \frac{1}{w^2}$ and $\epsilon_2 = 1 - \frac{4\pi}{w^3\tau}\sigma_{dc} \propto \frac{1}{w^3}$. In Fig 2.2, the variation of the optical conductivity and dielectric constant with frequency calculated by use of the Drude model is shown. In general, only the reflectivity and transmittance are accessible by optical experiments which can be evaluated via the optical constants n and k , i.e.,

$$R = \frac{(1 - n)^2 + k^2}{(1 + n)^2 + k^2} \quad (2.9)$$

and

$$T_r = 1 - (A + R) \quad (2.10)$$

Where R is the reflectivity, T_r is the transmission coefficient (transmittance), A is the absorption coefficient, n is the real part of the refractive index, and k is the imaginary part of the refractive index. From the reflectivity and transmission coefficients, the complex conductivity can be obtained via either the Fresnel formulas or Kramers Kronig analysis. The Kramers Kronig analysis is not always possible (e.g. due to a limited frequency range available for the measurement, or samples which are not opaque).

Within the framework of the Drude model, two frequencies are of important relevance: the scattering rate ($\gamma = \frac{1}{\tau}$) and the plasma frequency (w_p). This is because the scattering rate indicates how frequently electrons scatter, affecting electrical conductivity and energy loss, while the plasma frequency marks the transition between metallic reflection and optical transparency. This results in three spectral regimes being distinguished which are the Hagen Rubens regime for $w < \frac{1}{\tau}$, the relaxation or intermediate regime for $\frac{1}{\tau} < w < w_p$ and the transparent regime for $w > w_p$. Each of these three regimes has a characteristic optical response that is fundamentally different from the response found in other regimes. The Hagen Rubens regime is defined by the condition that $w\tau \ll 1$. In this regime, the optical properties are mainly determined by the dc conductivity (σ_{dc}) and the real part of conductivity (σ_1) is frequency independent, i.e., $\sigma_{dc} \approx \sigma_1(w) \gg \sigma_2(w)$. The real part of the dielectric constant is negative and large and both components of the refractive index are equal in this regime, i.e.

$$n(w) = k(w) \approx \left[\frac{\epsilon_2(w)}{2} \right]^{1/2} = \left(\frac{2\pi\sigma_{dc}}{w} \right)^{1/2} \quad (2.11)$$

The reflectivity in this regime can then be rewritten as:

$$R(w) = \frac{k(w) - 1}{k(w) + 1} \approx 1 - \left(\frac{2w}{\pi\sigma_{dc}} \right)^{1/2} = 1 - \left(\frac{8w}{w_p^2\tau} \right)^{1/2} = 1 - A(w) \quad (2.12)$$

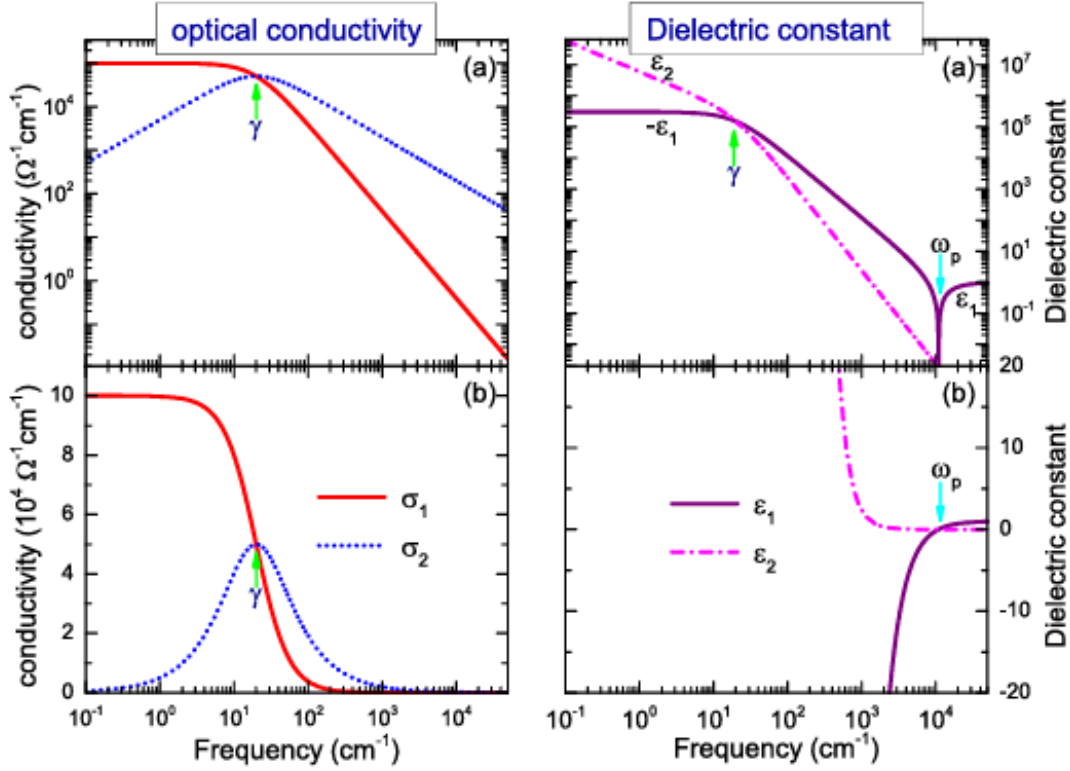


Figure 2.2: Frequency-dependent conductivity, σ , and dielectric constant, ϵ , calculated by use of the Drude model for a plasma frequency $\frac{w_p}{2\pi} = 1.1 \times 10^4 \text{ cm}^{-1}$ and $\frac{1}{2\pi\tau} = 20 \text{ cm}^{-1}$. The optical conductivity and dielectric constant are shown in (a) for a double-logarithmic and (b) for a semi-logarithmic scale. Below $\frac{1}{\tau}$, the real part of the optical conductivity, σ_1 , is nearly frequency independent and above $\frac{1}{\tau}$ it falls off with w^{-2} , while the imaginary part peaks at $\frac{1}{\tau}$. On the other hand, ϵ_1 is negative and independent of frequency below $\frac{1}{\tau}$. Above $\frac{1}{\tau}$, ϵ_1 decreases monotonically with frequency and becomes positive at higher frequencies. The frequency at which ϵ_1 changes sign (from negative to positive) is called the plasma frequency w_p . Further, the plasma frequency can also be interpreted as the frequency at which ϵ_1 and ϵ_2 cross each other.

Equation (2.12) is of paramount importance when it comes to the extrapolation of data to lower frequencies, as elaborated in the data-analysis chapter of this dissertation. Detailed information on Hagen-Rubens, relaxation, and transparent regimes can be found in [54].

2.1.2 Lorentz-Model

The optical properties of band semiconductors and insulators can best be described by the Lorentz model which describes the interaction of bound electrons with an external electromagnetic field. Unlike the Drude model (free electrons), Lorentz model accounts for electrons bound to ions, treating them as harmonic oscillators that experience a restoring, damping and driving force due to the external applied field. The motion of a bound electron under an external electric field $E(t)$ is:

$$m \frac{d^2 r}{dt^2} + m\gamma \frac{dr}{dt} + mw_0^2 r = -eE(t) \quad (2.13)$$

where m is the electronic mass, e is the electronic charge, $w_0 = \sqrt{\frac{k}{m}}$ is the natural resonance frequency for the electron, $\gamma = \frac{1}{\tau}$ is the damping coefficient, $E = E_0 e^{-i\omega t}$ is the external electric field and $r(t)$ is the displacement of the electron. Assuming a steady - state solution of the form $r = r_0 e^{-i\omega t}$ and solving Eq. (2.13) we get:

$$-mw_0^2 r_0 e^{-i\omega t} - im\gamma w r_0 e^{-i\omega t} + mw_0^2 r_0 e^{-i\omega t} = -eE_0 e^{-i\omega t} \quad (2.14)$$

Canceling the common factor $e^{-i\omega t}$ and solving for r_0 , gives:

$$r_0 = \frac{-eE_0}{m(w_0^2 - w^2 - i\gamma w)} \quad (2.15)$$

The macroscopic polarization P of a material due to the displacement of bound electrons within its atoms or molecules under an external electric field is given by $P = Ner$, where N is the number density of bound electrons. Substituting r_0 gives:

$$P = \frac{Ne^2}{m} \frac{-\epsilon_0}{w_0^2 - w^2 - i\gamma w} \quad (2.16)$$

Since the dielectric displacement field is defined as $D = \epsilon_0 E + P$ and where $D = \epsilon E$. This simplifies into the expression $\epsilon_0 E + P = \epsilon E$, substituting Eq. (2.16) into this expression gives:

$$\epsilon_0 + \frac{Ne^2}{m} \frac{1}{w_0^2 - w^2 - i\gamma w} = \epsilon \quad (2.17)$$

Thus the dielectric function becomes:

$$\epsilon(w) = 1 + \frac{w_p^2}{w_0^2 - w^2 - i\gamma w} \quad (2.18)$$

where $w_p^2 = \frac{Ne^2}{\epsilon_0 m} = \frac{4\pi n e^2}{m}$ is the plasma frequency and it describes the oscillator's strength.

The relationship between the conductivity and permittivity is given as;

$$\sigma(w) = -iw\epsilon_0(\epsilon(w) - 1) \quad (2.19)$$

substituting $\epsilon(w)$ into Eq (2.19) we get;

$$\sigma(w) = \frac{iw\epsilon_0 w_p^2}{w_0^2 - w^2 - i\gamma w} \quad (2.20)$$

By setting $w_0 = 0$, the drude description can be obtained from the lorentz description. Further from Eq. (2.20) the real and imaginary parts of the conductivity are:

$$\sigma_1(w) = \frac{\gamma w^2 \epsilon_0 w_p^2}{(w_0^2 - w^2)^2 + (\gamma w)^2} \quad (2.21)$$

$$\sigma_2(w) = \frac{w(w_0^2 - w^2) \epsilon_0 w_p^2}{(w_0^2 - w^2)^2 + (\gamma w)^2} \quad (2.22)$$

Unlike the Drude model, the reflectivity of the Lorentz model starts from a value different from 1, i.e., $R = |\frac{n-1}{n+2}|^2$. It increases at w_0 which can be related to the energy difference between two states or the energy gap of a semiconductor. The reflectivity drops at w_p which is the plasma frequency of these localized excitations. In the Lorentz model, three frequencies are of relevance which are $\frac{1}{\tau}$, w_0 and w_p giving way to four distinct regimes, i.e., the low-frequency regime for $w < (w_0 - \frac{1}{\tau})$, the absorption regime for $w_0 - \frac{1}{2\tau} < w < w_0 + \frac{1}{2\tau}$, the reflection regime for $w_0 - \frac{1}{\tau} < w < w_0$ and the transparent regime for $w > w_p$.

2.1.3 Extended Drude Analysis

The Drude model has frequently been used to describe the intraband optical transitions in solids. In this model, conduction electrons are considered to be a free electron gas while the remaining bound electrons and nuclei form a positive background. An obvious oversimplification with the Drude model is the assumption of the energy (frequency) independent scattering rate and electron band mass m . Although the Drude model has been used for a long time and it is frequently used today, there is need for modification, so that the frequency dependence of the scattering rate and electron band mass is taken into consideration. Several conducting materials, which are of current interest in the ongoing solid state physics research, are influenced by electron - electron interaction. This is particularly true in systems with d and f electrons, where the scattering of extended states with localized or narrowband states may occur and in materials deviating from the conventional Fermi liquid scenario. In such cases, it turns out that a simple Drude behavior assuming a constant scattering rate and band mass m is no longer appropriate. This calls for the necessity to extend the original Drude model to a more generalized formulation, the so called extended Drude model [58, 59], which takes into account the frequency dependence of the scattering rate, $\frac{1}{\tau}(w)$, and effective mass, $m^*(w)$. The extended Drude (or the generalized Drude) model satisfies the following equation:

$$\sigma(\hat{w}) = \sigma_{1D}(w) + i\sigma_{2D}(w) = \frac{w_p^2}{4\pi} \frac{1}{\Gamma(w) - iw \frac{m^*(w)}{m_b}} \quad (2.23)$$

with $m^*(w)$ being the effective mass and $\Gamma(w)$ being the scattering rate. By inverting Eq. (2.23), we get:

$$\Gamma(w) = \frac{1}{\tau(w)} = \frac{w_p^2}{4\pi} \frac{\sigma_{1D}(w)}{|\sigma_D|^2} \quad (2.24)$$

This relation is derived by inverting the complex conductivity, Eq. (2.23) and isolating the real part. The scattering rate represents the dissipative response resulting from collisions at a given frequency. It allows a direct evaluation of how carrier scattering evolves with frequency, reflecting interaction effects or disorder in the material.

Similarly, the frequency-dependent effective mass:

$$\frac{m^*(w)}{m_b} = \frac{w_p^2 \sigma_{2D}(w)}{4\pi w |\sigma_D|^2} \quad (2.25)$$

is obtained by isolating the imaginary part of the inverted conductivity. The frequency-dependent mass enhancement indicates how the carriers are renormalized due to many-body interactions, such as electron-electron or electron-phonon coupling. Both, Eq (2.24) and (2.25) are fundamental in analyzing optical data of strongly correlated materials, as they provide a more realistic and dynamic picture of charge carrier behavior than the conventional Drude model.

2.2 INTRODUCTION TO TOPOLOGICAL MATERIALS

Insulators are known to be non conducting because of a finite energy gap that separates the conduction and valence bands. Differences between insulators have been considered only quantitatively, such as in the band dispersion and the energy gap size. These insulators can be further classified into different classes according to the topology of their band structures [1-4]. For instance, the usual ordering conduction and valence bands of an ordinary insulator can be inverted by strong spin-orbital coupling (SOC), leading to topological insulators (TIs). The inverted bulk band structure topologically gives rise to metallic surface states. Therefore, TIs are characterized by gapless surface states inside the bulk energy gap. These surface states commonly exhibit a Dirac cone type dispersion in which spin and momentum are locked-up and perpendicular to each other. Topological insulator phenomena have been observed in many materials [5], such as HgTe [6, 7] and Bi₂Se₃ [8, 9]. The discovery of topological insulators (TIs) firmly established the notion of topology as a means to sharply distinguish electronic phases and classify quantum states of matter [1, 10]. Classification schemes based on the topology of the ground state wave function initially applied to electronic phases with an energy gap have since been extended to gapless systems [60]. This led to the identification of a new and special class of topological material known as the topological semimetals (TSMs). TSMs are characterized by a topologically stable Fermi surface originating from a crossing of energy bands. Band crossings of this kind can be associated with a topological number, which may depend on the symmetries responsible for enforcing or protecting the band crossing degeneracy. Different types of TSMs can be distinguished on the basis of key attributes of the band crossing, such as its degeneracy, the co-dimension

(i.e., whether the band degeneracy occurs at a point or on a line), and the dispersion in the vicinity of the crossing. Another possible distinction can be made on the basis of the origin of the crossing that is, whether it is symmetry enforced or arises as a result of a band inversion. These attributes, in combination with their topological characteristics, have led to the identification of a growing number of different TSM families, which include Dirac and Weyl semimetals [61], nodal line semimetals Ref. [18-20], type I and type II semimetals [21], multifold fermion semimetals [22, 26], and triple-point semimetals [23-25], among others. TSMs can host a variety of different low-energy excitations, which offer not only promising potential for future applications but also a new platform for the fundamental study of novel quasiparticles beyond the standard paradigm of known particles in high-energy physics [26]. Due to the nontrivial topology of the bulk and surface electronic states, TSMs are expected to exhibit intriguing quantum transport properties, such as unusual magnetoresistance and the chiral anomaly [27-32]. Furthermore, TSMs are of interest due to their potential future applications in chemical catalysis [31, 32], quantum computation and spintronic [33]. A particularly useful theme that makes these connections transparent is the notion of symmetry. The symmetry properties of solid-state materials are determined by their crystal and compositional structure and in turn determine the degeneracies and crossings of energy bands. Symmetry therefore naturally relates structural and electronic characteristics. As a result, the symmetries of the crystal lattice, i.e., the symmetries of the space group in combination with time-reversal or inversion symmetries, are of fundamental importance for TSMs and provide an important underpinning for the theory of TSMs.

2.2.1 Weyl Semimetal

The Dirac Hamiltonian plays a crucial role in the theory of topological materials. Its significance follows from the fact that, in the presence of time-reversal or inversion symmetry, a three-dimensional Dirac fermion appears at the topological phase boundary between a normal insulator and a TI [34]. To illustrate this in more detail, consider the Dirac Hamiltonian in three dimensions given by.

$$H(k) = \begin{pmatrix} m & vk \cdot \sigma \\ vk \cdot \sigma & -m \end{pmatrix} = vk \cdot \sigma \tau_x + m \tau_z \quad (2.26)$$

Where $k = (k_x, k_y, k_z)$ is momentum, v is the Fermi velocity and m is mass. $\sigma = (\sigma_x, \sigma_y, \sigma_z)$

and $\tau = (\tau_x, \tau_y, \tau_z)$ are the two sets of Pauli matrices, which can be viewed as spin and orbital degrees of freedom, respectively. The mass parameter m controls the topological transition. When m is tuned such that it changes sign, the topology of the ground state changes. A sign change of m in Equation (2.26) corresponds to a band inversion of a time-reversal symmetry invariant momentum and thus describes the transition between a normal insulator and a TI. At the critical point of the transition, defined by $m = 0$, the spectrum of Equation (2.26) is gapless at $k = 0$, giving rise to a fourfold - degenerate point node with linear dispersion. As a result, at the critical point the low-energy electronic excitations are governed by a massless Dirac equation which decouples into two separate equations given by $\pm v k \cdot \sigma$, where each equation describes a two-component chiral Weyl fermion with chirality ± 1 . Weyl semimetals (WSMs) are a recently realized class of topological materials which stems from the massless Dirac Hamiltonian equation, in the ideal case, WSMs have low energy excitations that behave like relativistic Weyl fermions [62]. These fermions are solutions to a massless version of the Dirac equation:

$$i\hbar\gamma^\mu\partial_\mu\psi = 0 \tag{2.27}$$

(Where γ^μ are the Dirac matrices) which was originally considered by Hermann Weyl in 1929 [63]. In addition to being massless, Weyl fermions have a definite chirality, meaning that the spin and momentum are locked parallel or anti-parallel to one another [62, 63]. Weyl fermions are thus said to come in one of two types: right- or left-handed, depending on the relative direction between the spin and momentum. In their condensed matter realization, Weyl fermions exist as quasi particle excitations in the vicinity of so-called Weyl points [64], which are band crossings with linear dispersions in three-dimensions that act as monopoles of Berry curvature.

A well-known theorem from Neumann and Wigner states that energy crossings between bands of the same symmetry are generally forbidden [16]. Avoided crossings, as they are known, results from interactions between the two bands which lift the degeneracy and produce a band gap. However, as shown by Herring in 1937 [65], band degeneracies unrelated to specific symmetries may occur in systems of three or higher spatial dimensions. As noted above, these band crossings act as monopoles of the Berry curvature. The transformation properties of the Berry curvature under two fundamental symmetries: time-reversal and inversion, will determine whether a material can support the existence of Weyl points. Under

time-reversal symmetry the Berry curvature transforms as [66];

$$\Omega_n = -\Omega_n(-k) \quad (2.28)$$

While under inversion symmetry it transforms as:

$$\Omega_n = \Omega_n(-k) \quad (2.29)$$

It is clear from these relations that if a material possesses both time-reversal and inversion symmetry that the Berry curvature will be zero throughout the entire Brillouin zone (BZ). To support a non-zero Berry curvature a material must therefore break either time-reversal or inversion symmetries. In addition to this, the fermion doubling theorem of Nielsen and Ninomiya states that Weyl points must come in pairs of opposite chirality [63, 67-68]. In other words, the number of sources and sinks of Berry curvature in the BZ must be the same. If a material system breaks time-reversal symmetry, we thus find that the minimum possible number of Weyl points will be two: one left and one right chiral point. On the other hand, if a material breaks inversion symmetry we find that the minimum number of points must be four. In the vicinity of the Weyl points the dispersion relation may be obtained from the Hamiltonian in Eq. (2.27) as:

$$E_n = \pm \hbar v F k \cdot \sigma \quad (2.30)$$

The dispersion is linear in momentum in all three directions, with the spin polarized parallel or anti-parallel to the momentum. In the ideal case, the Weyl points are located at the Fermi level and there are no other topologically trivial bands coexisting at the Fermi level. However, finding such materials presents a challenge [68], since many WSM have trivial bands that also cross the Fermi energy [69], or have Weyl points that are located far from the Fermi level [70]. The family of compounds (Nb,Ta)(P,As) were the first theoretically predicted inversion symmetry-breaking WSMs [47] to be experimentally confirmed. Angle-resolved photoemission spectroscopy measurements of the bulk and surface band structures revealed the presence of Weyl points and surface Fermi arcs [44], and transport measurements presented evidence for the chiral anomaly [71-73] (although debate arose whether the

negative magnetoresistance taken as evidence for the chiral anomaly could have been due to non-topological effects such as current jetting [30]). Since 2015 numerous other WSM have been identified, [62, 68, 74]. In a type-I WSMs the constant energy cross section of the Weyl cone shrinks to a point as the energy is swept through the Weyl point. In contrast, for type-II WSMs the constant energy surface does not become point-like at the energy of the Weyl point due to the intersection of the electron and hole pockets that form the point [75]. The Weyl cones of a type-II WSMs are therefore tilted versions of type-I Weyl cones.

2.2.2 Type I and II Weyl Semimetal

Metals can exhibit nontrivial topological features [21] of which the ones with vanishingly small density of states at the Fermi level, known as semimetals (SM), stand out. For these, a distinction between topologically protected surface and bulk metallic states can still be made, and their Fermi surfaces (FS) exhibit a topological (T) characterization. Two kinds of TSM that have attracted special attention are Dirac and Weyl semimetals. In these materials a linear crossing of two (Weyl) or four (Dirac) bands occurs at the Fermi level (see the left panel of Fig. 2.3. The effective Hamiltonian for these Weyl or Dirac band crossings is given by the Weyl or gapless Dirac equation, respectively. The Weyl crossings are protected from gapping, a statement of the massless nature of the Weyl fermion. The appearance of Weyl points (WPs) is only possible if the product of parity and time-reversal (TR) is not a symmetry of the structure. When present, a WP acts as a topological charge, either a source or a sink of Berry curvature. A Fermi surface (FS) that surrounds a WP has a well-defined Chern number, corresponding to the topological charge of this point. Since the net charge has to vanish in the entire Brillouin zone (BZ), WPs always come in pairs; WPs are stable to weak perturbations and can only be annihilated in pairs of opposite charge. A large number of unusual physical phenomena are associated with WSMs including the existence of open Fermi arcs on the surface [16, 76], and different magnetotransport anomalies [77–81]. WSMs with broken TR symmetry have been predicted to exist in several materials [30, 76, 82], but experimental verification has been lacking. More recently, the WSM was predicted to exist in inversion-breaking single crystal non-magnetic materials of the TaAs class [17, 83]; this prediction was soon verified experimentally [45, 84]. Up until now, WSMs have been thought to have a point-like FS at the WP and are referred to as type I WPs (WP1), to contrast them with the new type II WPs (WP2) that exist at the boundary of electron and hole pockets, as illustrated in the right panel of Fig. 2.3. (c) and (d).

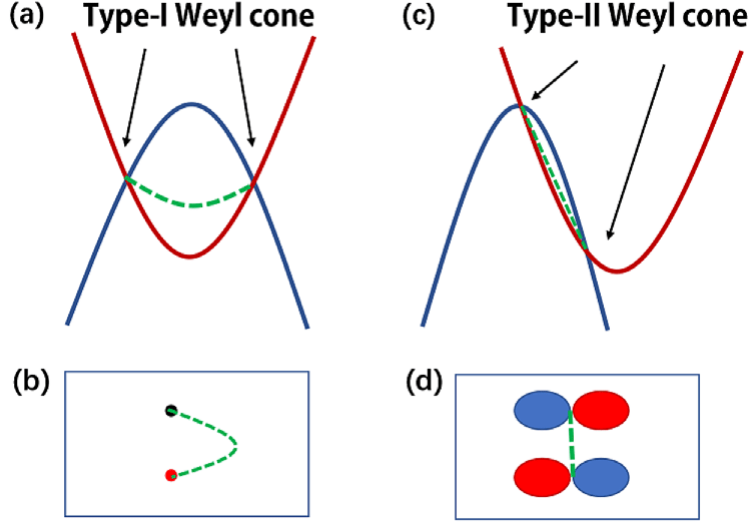


Figure 2.3: Type - I and type - II Weyl semimetals (a) A sketch of the e-k dispersion of a type-I Weyl semimetal which can be viewed as a negative direct bandgap semiconductor. The type-I Weyl nodes exist at the crossing points where the conduction band (red) and valence band (blue) dip into each other. A Fermi arc (green dotted line) connects the pair of Weyl nodes. (b) The Fermi surface (Fs) on the surface of a type-I Weyl semimetal as depicted in (a). The Fermi level is located at the energy of the Weyl nodes. Bulk Weyl cones are projected onto the surface as two discrete points (red, blue) connected by a Fermi arc surface state (dotted green line). (c) A sketch of e-k dispersion of an inversion symmetry breaking type-II Weyl semimetal which can be viewed as a negative indirect bandgap semiconductor. Tilted type-II Weyl cones form at the intersection of conduction and valence bands. (d) Fs on the surface of a type-II Weyl semimetal as depicted in (c). Inversion symmetry breaking constrains the minimum number of Weyl nodes to be four. Here, the Fermi level is assumed to cut at the energy of the lower Weyl node in (c). Projected bulk electron (red) and hole (blue) pockets coexist on the surface Fs and touch at one discrete point, the type-II Weyl nodes. A Fermi arc (green dotted line) connects one pair of projected Weyl nodes. Picture from [86].

WSMs type I respects Lorentz symmetry, while type II, does not [85]. The TaAs family of WSMs exhibits ideal Weyl cones in the bulk band structure and belongs to the type-I class, i.e., the FS shrinks to a point at the Weyl point. More recently, type-II WSMs have been proposed to exist in the layered transition-metal dichalcogenides WTe_2 [85] and its sister compound MoTe_2 [21]. Here, the Weyl cone exhibits strong tilting so that the Weyl

point is the contact point between an electron pocket and a hole pocket in the FS. Type-II WSMs are expected to show very different properties from type-I WSMs, such as anisotropic chiral anomaly depending on the current direction and a novel anomaly hall effect (AHE)[85].

2.2.3 Tungsten Diphosphide, WP_2

WP_2 is a three dimensional compound which crystallizes in a non-symmorphic $\text{Cmc}2_1$ space group. In this orthorhombic structure, tungsten atoms are surrounded by seven P atoms, six located at the corners of the triangular prism and the seventh outside one of the rectangular faces. As can be seen in Fig. 2.4 (a) the compound contains a mirror plane perpendicular to the a-axis, a c-glide perpendicular to the b-axis and a two-fold screw axis along the c-axis. Interestingly, the space group symmetry of WP_2 is very similar to the two dimensional WTe_2 which also contains a mirror- plane, a glide-plane and a two-fold screw axis. Fig. 2.4 (b) shows a typical crystal of WP_2 which is needle-shaped with its length oriented along the a-axis orientation. Interestingly, the space group symmetry of WP_2 is very similar to the two dimensional WTe_2 which also contains a mirror- plane, a glide-plane and a two-fold screw axis. Fig. 2.4 (b) shows a WP_2 needle-shaped crystal oriented along the a-axis.

Recently, WP_2 was theoretically predicted to be a type II WSM that hosts four pairs of Weyl points with opposite chirality located below the Fermi level [47]. The distance between the two Weyl points of each pair in momentum space is so long that the nearest Weyl points have the same chirality. Since the positions of the Weyl points are sensitive to the small perturbations of the crystal structure, such as structural distortions and defects, and the two Weyl points with opposite chirality would annihilate if they meet in momentum space, the same chirality of the neighboring Weyl points makes the predicted type-II WSM state of WP_2 particularly robust against structural distortions or defects. This distinguished character of the protection of the neighboring Weyl points with the same chirality against annihilation upon structural distortions or defects significantly reduces the probability of scattering between the neighboring Weyl points and thereby playing an important role in the extremely low resistivity observed in WP_2 [87].

Fig. 2.4 (c) depicts how a four-fold degenerate Dirac point can be split into two Weyl points with opposite chirality via inversion symmetry breaking (or alternatively in a magnetic field). In the absence of spin orbit coupling (SOC) WP_2 possess two pairs of four-fold degenerate linear band crossing points with opposite sign of Chern numbers ± 2 . The Chern number is

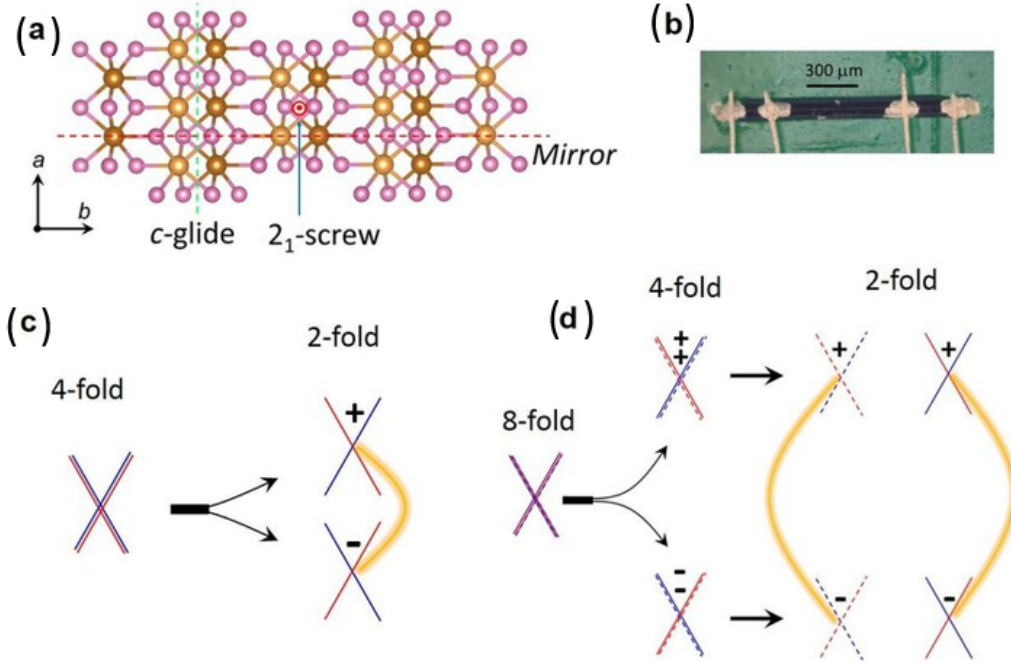


Figure 2.4: (a) Non-symmorphic crystal structure of WP_2 (W and P atoms are denoted by brown and pink spheres, respectively). For clarity, W atoms on the upper ab -plane are denoted by light brown spheres and the W atoms on the ab -plane displaced by half of the unit cell along the c -axis are denoted by dark brown spheres. Red and green dashed lines are the positions of the mirror and glide plane, respectively. Screw-axis along the c -axis is shown by red dot. (b) A needle shaped single crystal of WP_2 with the length, depth and width along a , b and c -axis. (c) Splitting of a four-fold degenerate Dirac point with zero Chern number into 2 two-fold degenerate Weyl points of opposite chirality on symmetry breaking. (d) The neighbouring Weyl points in WP_2 have same chirality. This kind of Weyl point can be viewed as the splitting of an 8-fold degenerate point without inclusion of SOC. On reducing the symmetry, the 8-fold linear crossing split into a pair of 4-fold degenerate points with opposite Chern numbers of $C = \pm 2$, which is just the overlap of two Weyl point with same chirality. SOC just lifts the overlap of two Weyl points in k -space. Since the Weyl points with opposite chirality are relatively far away from each other, they are more robust and the Fermi arcs are longer than that formed in normal Weyl semimetals picture taken from [87].

the integral of the Berry curvature around a particular point in momentum space. When SOC is introduced, the spin degeneracy is lifted so that the linear band crossing points evolve into two $\times$ two-fold degenerate linear band crossing Weyl points of the same chirality. The fact that they have the same chirality means that they are robust (see Fig. 2.4(d)). This makes WP_2 unique which differs from other Weyl semimetals.

Chapter 3

METHODOLOGY

To accomplish the task of optical investigation of WP_2 , various experiments had to be done. First the sample was grown and characterized after which resistivity and infrared optical spectroscopy measurements were done. In the next section a brief description of the investigated sample and the experiments that were done.

3.1 Growth and structure characterization of WP_2 single crystals.

High-quality WP_2 single crystals were grown by chemical vapor transport method. P, WO_3 , and I_2 were mixed and sealed in a quartz tube under a vacuum, then the WP_2 crystals were grown in a two-zone furnace with a temperature gradient of 1000 °C (source) to 900 °C (sink) for 10 days. Crystal and surface structures were characterized by X-ray diffraction (XRD), transmission electron microscopy, and scanning tunneling microscopy. As shown in Fig. 3.1 (b), the as-grown WP_2 single crystals possess several natural crystal faces parallel to the a-axis including the (010), (062), and (021) surfaces. The optical responses for E//a and E//c can be measured on the (010) surface, whereas the response for E//b cannot be directly measured on these three surfaces. In order to measure the complete optical response of WP_2 , it is imperative to fabricate other simple crystal faces with low indices, such as the (001) surface, which can be used to measure the optical response for E//b. Using X-ray Laue photography, the crystals were carefully oriented and cut into small pieces along the appropriate crystalline axes to obtain the (001) surface. In this dissertation WP_2 samples were investigated by Resistivity and Polarized Fourier-transform infrared spectroscopy measurements were performed with a Fourier-transform infrared spectrometer (Bruker Vertex

80v) at the University of Stuttgart in Germany

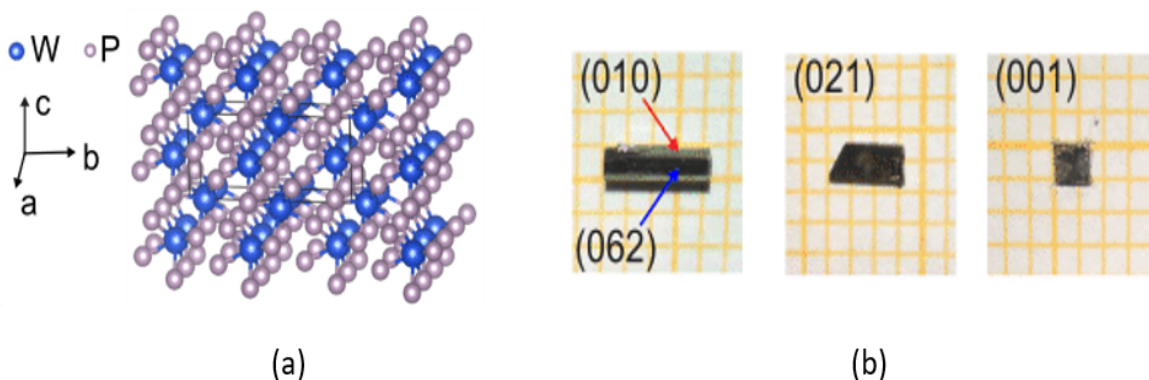


Figure 3.1: Structure characterizations of WP_2 . (a) Crystallographic structure. The black lines indicate a unit cell. (b) Optical images of the samples with different crystalline surfaces adopted for XRD and optical reflectance measurements [88]

3.2 Fourier-transform infrared spectroscopy (FTIR)

Fourier-transform infrared spectroscopy (FTIR) is a powerful and commonly used technique for identifying chemical compounds and understanding their molecular structure. It works by measuring how a sample absorbs infrared light at different wavelengths, revealing the detailed information about the various functional groups. The infrared radiation is focused on the sample where it is either transmitted (transmittance) or reflected (reflectance). Apart from reflection and transmission, some of the incident infrared radiation is absorbed by the sample. The resulting spectrum is like a fingerprint; no two materials produce the same infrared spectrum, making infrared spectroscopy a useful tool for several types of analysis. With FTIR spectroscopy, all of the infrared frequencies arriving at the detector are measured simultaneously, rather than individually as is the case with dispersive elements. This is achieved by employing an interferometer producing a unique signal. The signal can be measured very quickly, usually on the order of a second or so. Most interferometers employ a beam splitter, which divides the incoming infrared beam into two optical beams. One beam reflects off a flat mirror which is fixed, while the other beam reflects off a flat mirror that can be moved over a short distance (typically a few millimeters). The two beams

are recombined when they meet back at the beam splitter. Due to the different optical lengths these two beams interfere with each other and the resulting interferogram has the unique property that every data point (a function of the moving mirror position, Δx), has information about every infrared frequency, which comes from the source. This means that as the interferogram is measured, all frequencies are being measured simultaneously. By employing a Fourier transformation the desired spectral information for further analysis is obtained.

The normal instrumental process is as follows:

- Infrared radiation is emitted from a source. These sources can be a mercury lamp for far-infrared (FIR), globar for mid-infrared (MIR), or a tungsten lamp for near-infrared (NIR) measurements. The radiation passes through an aperture which controls the amount of energy reaching the sample and, ultimately, the detector.
- In the interferometer the spectral encoding takes place. At the sample the radiation is transmitted or reflected, depending on the type of analysis being accomplished.
- Finally, in the detector interferogram is measured. The detectors used are bolometers for the FIR signal, MCT (mercury cadmium telluride) detectors for the MIR signal, and InSb (indium antimonide) detectors for the NIR signal.
- The measured signal is digitized and Fourier transformed.

To obtain absolute values for the transmittance or reflectance, a background spectrum has to be measured. This background spectrum usually is a measurement with no sample in the optical path which is in turn compared to the measurement with sample. This technique results in a spectrum, which has all of the instrumental characteristics removed. Some of the major advantages of FTIR spectroscopy include speed, sensitivity, mechanical simplicity, and internal calibration achieved by employing a HeNe laser. These advantages, along with several others, make measurements made by FTIR spectroscopy accurate and reproducible. With Fourier-transform spectroscopy, experiments in the far-infrared (FIR) regime [$10 - 500 \text{ cm}^{-1}$], mid-infrared (MIR) regime [$500 - 4000 \text{ cm}^{-1}$], near infrared (NIR) regime [$4000 - 14\,000 \text{ cm}^{-1}$], and NIR to visible range [$14\,000 - 22\,000 \text{ cm}^{-1}$] could be performed. The frequency range from 10 cm^{-1} to $14\,000 \text{ cm}^{-1}$ is called infrared frequency regime and the spectroscopy done in this frequency range is referred to as infrared spectroscopy. Depending on the frequency range of interest, different combinations of sources, optical windows, filters, beam splitters, detectors, etc. are used to carry out the experiment. Experiments for the far-far-far infrared (FFFIR), far-far-infrared (FFIR), far infrared (FIR), MIR, NIR, and NIR

to visible range have been performed. A summary of the combinations used for the various frequency ranges is outlined in table 3.1.

Table 3.1: Various combinations for the measured frequency ranges of the Fourier-transform spectroscopy experiment.

Frequency Range cm^{-1}	Beam Splitter	Source	Detector	Optical Window	Filter	Saturation Signal
FFFIR 15 - 60	50 μm thick Mylar	Mercury Lamp	1.5 K pumped Silicon bolometer	Mylar PP/PE	Black poly	32768
FFIR 30 - 20	23 μm thick Mylar	Mercury Lamp	1.5 K pumped Silicon bolometer	Mylar PP/PE	Black poly	32768
FIR 40 - 700	Silicon Mylar	Mercury Lamp	4.5 K pumped Silicon bolometer	Mylar PP/PE	Black poly	32768
MIR 500 - 8000	KBr	Global	77 K MCT	KBr	Grid	5000
NIR 2000 - 11 000	CaF ₂	Tungsten Lamp	77 K Insb	KBr	-	32768
NIR - Visi- ble 9000 - 22 000	CaF	Xenon arc Lamp	Silicon/GaInAs detector	CaF	-	80000

It should be emphasized that due to time constraint and financial challenges only measurements starting from MIR up to NIR-Visble were done for the current research presented here, using Bruker Vertex 80v spectrometer. The Bruker Vertex 80v spectrometer is a high-performance Fourier transform infrared (FTIR) spectrometer that offers several advantages over other spectrometers. It provides high spectral resolution of up to 0.06 cm^{-1} , high sensitivity, and a wide spectral range of $30,000 - 50\,000\text{ cm}^{-1}$, making it suitable for a broad range of applications. The spectrometer features advanced beam splitter design, high-speed scanning capabilities, and advanced software for data analysis and processing. Fig. 3.2 shows sketches of the layouts of the Bruker spectrometers.

To measure reflectivity and transmission at various temperatures, the sample is placed in a cryostat. In this research work, for reflectivity measurements, a continuous flow cryostat with a gold evaporation unit was used. To get absolute reflectivity free from instrumental artifacts, gold or silver depending on the frequency range of interest is evaporated on the sample in the second run of the experiment. The reflectivity of the sample coated with gold or silver is used as reference. The absolute reflectivity (R) is then given by:

$$R = \frac{R_{sample}/R_{mirror}}{R_{Ag,Au}/R_{mirror}} \approx \frac{R_{sample}}{R_{Ag,Au}} \quad (3.1)$$

With $R_{Ag,Au}$ being the reflectivity of the sample coated either with gold or silver.

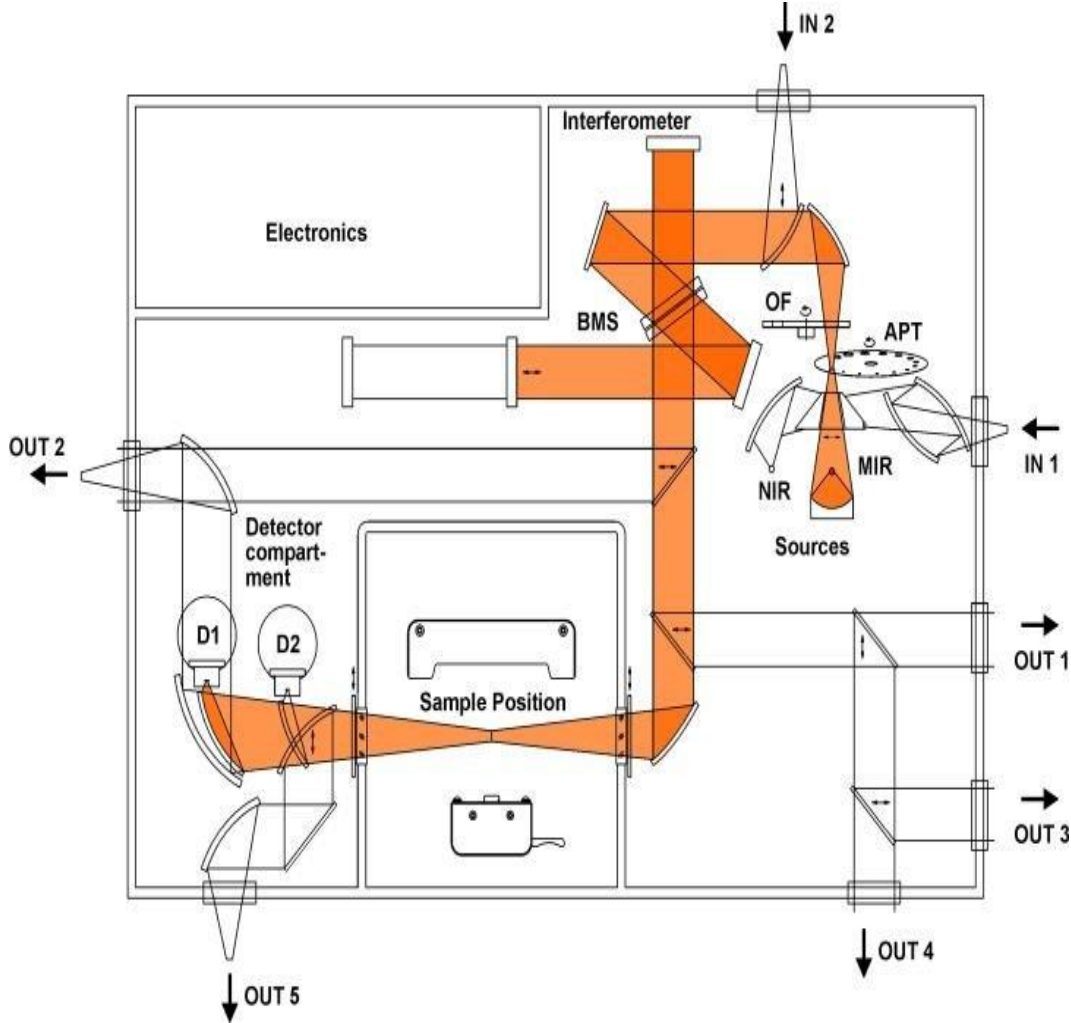


Figure 3.2: Optical path layout of the Bruker Vertex 80v [106]

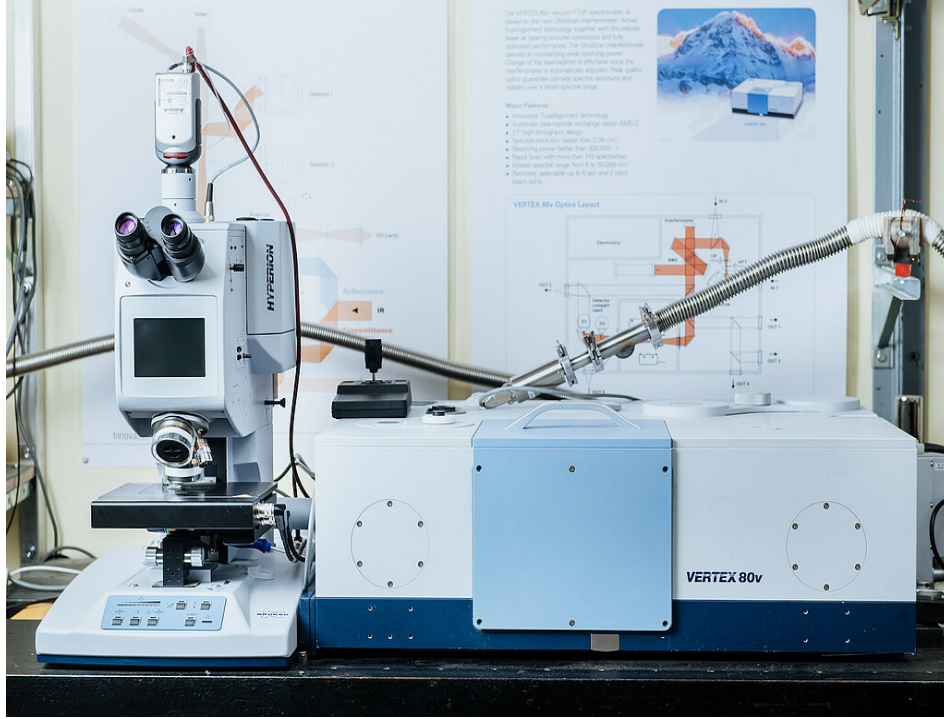


Figure 3.3: Bruker Vertex 80v with a microscope used in reflectivity measurements picture taken from [107]

The Vertex 80v's are mechanically designed to provide high stability and precision, ensuring high-quality spectra and reliable operation. The instrument is built on a rigid, vibration-isolated platform to minimize mechanical noise and interference.

The design of the Vertex 80v consists of the following components:

- **Interferometer Chamber:** The interferometer chamber is a critical component of the Vertex 80v, housing the beam splitter, mirrors, and delay line. The chamber is evacuated to a high vacuum to minimize atmospheric interference.
- **Optical Bench:** The optical bench is a rigid, vibration-isolated platform that supports the interferometer chamber and other optical components.
- **Sample Compartment:** The sample compartment is designed to hold the sample and provide a stable, temperature-controlled environment. The compartment is equipped with a temperature controller and a sample holder. interferometer chamber and other optical components.
- **Electronics:** The electronics of the Vertex 80v are designed to provide high-speed

data acquisition and processing. The instrument is equipped with a high-performance computer and advanced software for data analysis and processing.

The Vertex 80v uses a Michelson interferometer, which is a type of FTIR spectrometer. The Michelson interferometer is a common design used in FTIR spectroscopy, known for its high spectral resolution and sensitivity. The Michelson interferometer works by splitting the infrared radiation into two beams, one of which passes through the sample and the other serves as a reference beam. The two beams are then recombined, creating an interference pattern that is detected by the detector. The interference pattern is then converted into a spectrum using a Fourier transform algorithm. The Vertex 80v uses a high-sensitivity, liquid-nitrogen-cooled MCT detector, which provides high sensitivity and low noise. The MCT detector is a type of photovoltaic detector that converts the infrared radiation into an electrical signal. The MCT detector is cooled to a temperature of 77 K using liquid nitrogen by a closed – cycle cryostat, which reduces thermal noise and increases sensitivity. The detector is also equipped with a cold filter to reduce thermal radiation and improve signal-to-noise ratio.

3.3 Resistivity Measurements

The electrical resistivity measurements were measured using an in house built University of Stuttgart PI1 (First Physikalisches Institute) resistivity measurement device. The electrical resistivities were measured using a standard four-probe method with the electric currents applied along the a-axis. Figure 3.4 shows a simple sketch for a sample to be used for a four point probe resistivity measurements. These electrical leads were in turn attached to the adapter which was in turn mounted onto the sample holder. The sample holder was then mounted into the cryostat.

The cryostat was evacuated and necessary parameters/ the sequence for the measurements loaded in the computer/ controller. The necessary parameters included the current to be used for the measurements, the sample dimensions in millimeters, the Proportional-Integral-Derivative (PID) values etc. After carrying out the room temperature resistivity test measurements to ensure that the contacts were properly fixed, the experiment was started and resistivity was measured using a current of 5.0 mA at temperatures ranging from room temperature down to 2 K.

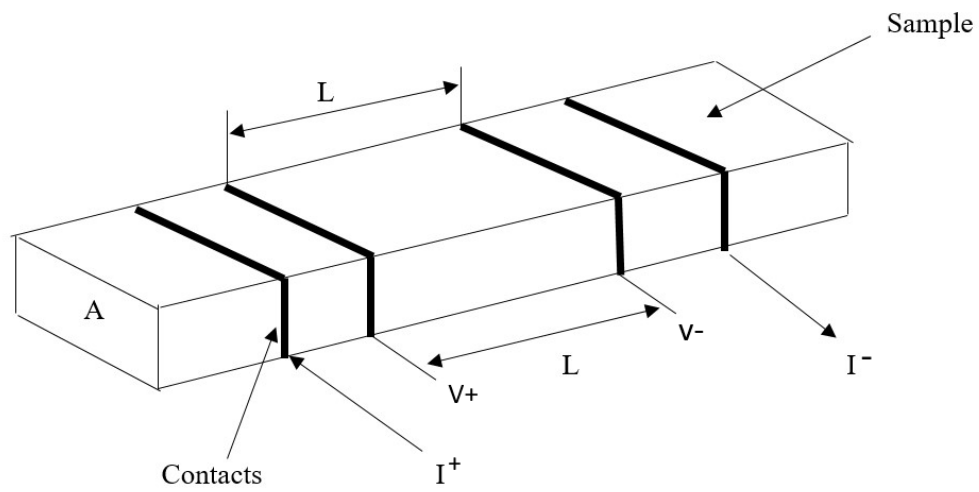


Figure 3.4: sketch of a sample attached to the electrical leads. A is the cross section area, I is the current input contact, L is the distance between the voltage input contacts.

Chapter 4

DATA ANALYSIS

4.1 ANALYSIS OF REFLECTIVITY DATA

Kramers - Kronig analysis is a powerful tool for obtaining optical constants from reflectivity measurements. This analysis can only work well if the reflectivity data is collected from zero to very high frequencies. Hence, to investigate a material by optical reflectivity means, data needs to be collected over a wide range of frequencies using different radiation sources, optical windows, filters, and detectors such as outlined in table 3.1. First, the measured data at each temperature need to be merged for different frequency ranges i.e. MIR, NIR and room temperature NIR - visible measurements. Second, extrapolation at low and high frequencies need to be done, after which Kramers-Kronig analysis is performed to obtain the optical conductivity and dielectric constant from the reflectivity data. The optical conductivity obtained from Kramers-Kronig and the merged reflectivity are then fitted using the Wasf program with drude - Lorentz contributions. The fitted reflectivity is smoothed and a second Kramers-Kronig analysis is then applied on it. Below is a brief explanation of the various steps involved in reflectivity-data handling.

4.1.1 Merging of reflectivity data

For Kramers-kronig analysis to work, reflectivity data has to be collected over a wide range from zero to $400\,000\text{ cm}^{-1}$.i.e. closed loop with reflectivity at the highest being approximately equal to zero, hence the need for merging and extrapolation. As for WP₂ single crystals the measurements were done in three steps i.e. MIR, NIR, and room temperature NIR – Visible measurements. Figure 4.1 (a) illustrates an example of the overlapping area of the reflectivity for E//c - axis plane measured in two frequency regime i.e. for NIR and

VIS data set at 300 K temperature measurements which were merged together.

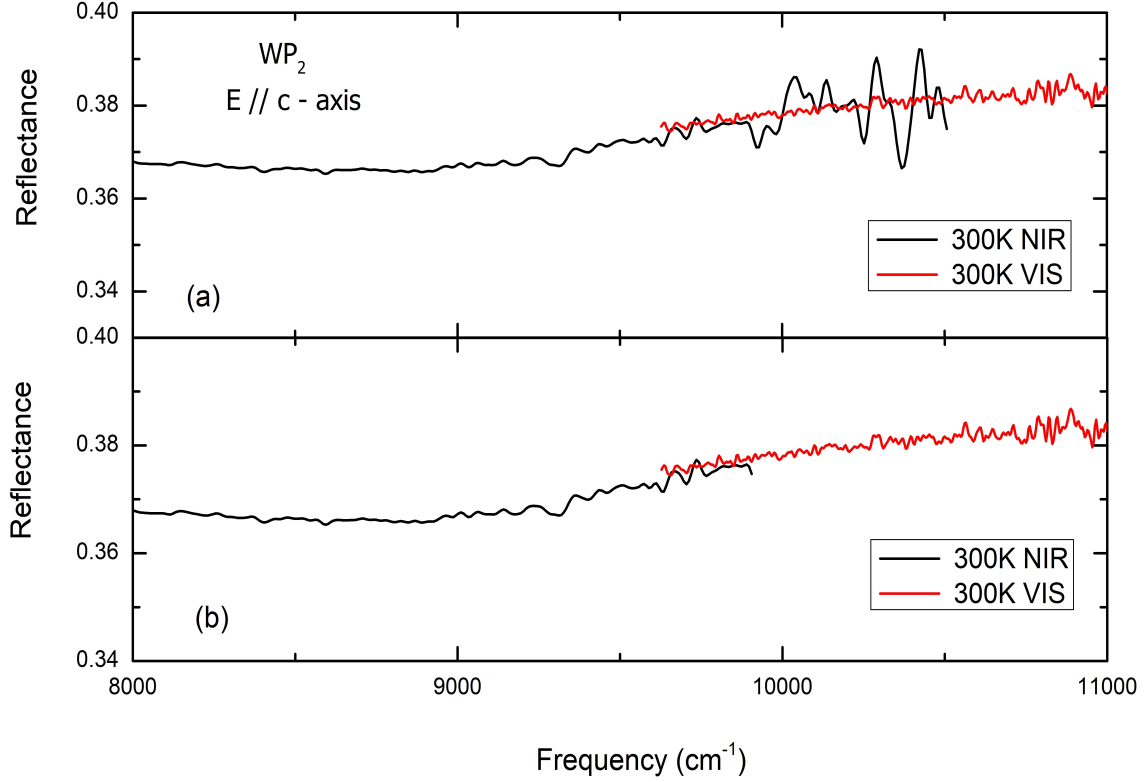


Figure 4.1: showing (a) 300 K (i.e. NIR and VIS ranges) reflectivity independent measurements for WP_2 which are to be merged. (b) shows the same two measurements but with noise cut off. The noise in (a) between 10 000 – 10 500 cm^{-1} due to the silicon beam splitter, has to be cut before Kramers - Kronig calculations.

One can clearly observe that the connection between the two measurements is very good, which is an indication of reliable measurements. The small difference in the intensity can be attributed to different alignment for these experiments. Before merging the data set noise fluctuations at the range edges were cut off from each of the measured frequency ranges as illustrated in figure 4.1 (b).

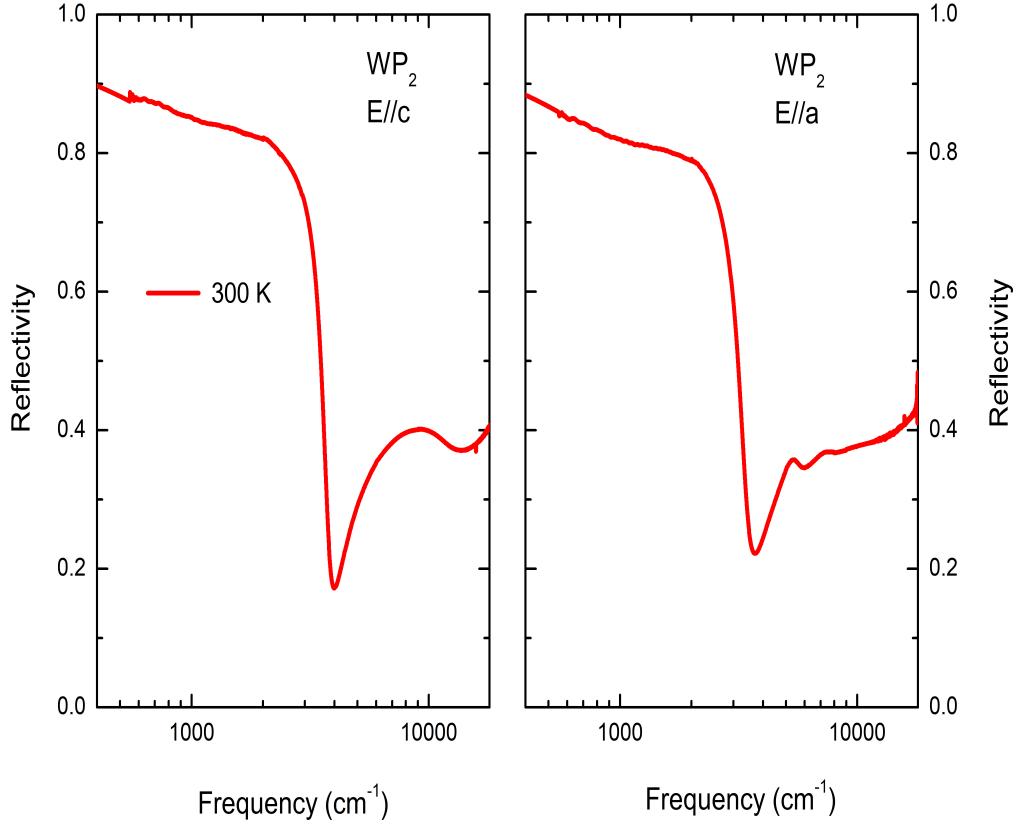


Figure 4.2: showing merged reflectivity measurement for WP_2 of incident light applied along its crystalline c-axis and a-axis plane over a wide range of frequencies for 300 K.

4.1.2 Data extrapolation

Extrapolation is imperative in experimental situations where data is only available over a limited range of frequencies or wavenumbers to accurately predict the behavior of the response function outside of the measured range over which the Kramers- Kronig relations are applied. To apply the Kramers-Kronig analysis reflectivity data should be available from zero frequency up to a frequency where the reflectivity of the sample is almost zero. Since in the measurements the frequency range was limited to frequencies between 540 cm^{-1} and $20\,000 \text{ cm}^{-1}$, the measured data needed to be extrapolated at both low and high frequencies. At high frequencies ($\omega \rightarrow \infty$) the reflectivity goes to zero. The extrapolation for high frequencies was done using the XRO (x-ray optical) data calculation. This involved drawing of data at higher frequency using the phase data from XRO calculation and extrapolating it according to the relation;

$R(w) = \{R_1 \times \left(\frac{w_o}{w}\right)^2 \text{ for } 20\,000 \text{ cm}^{-1} \leq w \leq 80\,000 \text{ cm}^{-1} ; w_o = 20\,000 \text{ cm}^{-1}\}$
 With R_1 being the reflectivity at $20\,000 \text{ cm}^{-1}$ (the highest measured frequency). To this end, the low-frequency extrapolations of the reflectivity data were based on the Drude-Lorentz fitting.

4.1.3 Kramers-Kronig Analysis

The real and imaginary parts of the complex response functions are not independent but are related to each other by Kramers-Kronig relations which were first given in 1926 by Kramers [89] and Kronig [90]. The Kramers-Kronig relations play an important role not only in the theory of response functions [91], but also enables the evaluation of the components of the complex conductivity and dielectric constant when only one optical parameter, e.g. the reflected power, is measured. With $R(w)$ obtained over a wide range of frequencies as outlined above, the Kramers-Kronig analysis can be utilized to evaluate the phase, $\varphi_r(w)$. Having the reflectivity and the phase, other optical parameters (e.g. the complex conductivity, dielectric constant, etc.) can be calculated. In practice, for the Kramers-Kronig analysis to be successful, the data must cover a wide frequency range and the sample must not be transparent. Such an analysis was applied to the reflectivity of WP_2 due to the fact that the investigated single crystal is not transparent and the reflectivity data cover a wide frequency range. The merged and extrapolated data is loaded in the kramers - kronig program, which is run to calculate the real part of the complex conductivity (σ_1). Knowing this parameter the imaginary part of the complex conductivity can be calculated using relationships in table 2.1.

The complex reflectivity fed into the kramers-kronig program was in the form:

$$\hat{r}(w) = |\hat{r}(w)| e^{i\Phi(w)} \Leftrightarrow \ln \hat{r}(w) = \ln |\hat{r}(w)| + i\Phi(w) \quad (4.1)$$

Where the measured reflectivity signal is $R(w) = |\hat{r}(w)|^2$ and $\Phi(w)$ is the phase shift between incident and reflected light and is given by:

$$\Phi(w) = \frac{w}{\pi} \int_0^\infty \frac{\ln[R(w')] - \ln[R(w)]}{w^2 - w'^2} dw' \quad (4.2)$$

So having the reflectivity and phase shift, Kramers-Kronig program calculates the real part of the optical conductivity using the equation:

$$\sigma_1(w) = \frac{w}{4\pi} \frac{4\sqrt{R(w)}[1 - R(w)]\sin\Phi(w)}{[1 + R(w) - 2\sqrt{R(w)}\cos\Phi(w)]^2} \quad (4.3)$$

and the complex dielectric constant using relations outlined in table 2.1. By Kramers-Kronig relations, the imaginary part of the optical conductivity is readily obtained:

$$\sigma_2(w) = \frac{w}{4\pi} \left(1 - \frac{[1 - R(w)]^2 - 4\sqrt{R(w)}\sin^2\Phi(w)}{[1 + R(w) - 2\sqrt{R(w)}\cos\Phi(w)]^2} \right) \quad (4.4)$$

4.1.4 Fitting of reflectivity and conductivity data

Various programs to model the reflectivity or transmission data are available. In this dissertation, a shareware fit program called WASF program provided by University of Stuttgart was utilized to model the measured data set. The reflectivity data, as well as the calculated conductivity for single crystals, are fed into the program where they are fitted with various Drude-Lorentz components. The reflectivity and conductivity spectra are fitted with one drude to mimic itinerant electrons, and a number of Lorentz oscillators to mimic interband transitions, phonons, as well as localized carriers, etc. The two fit parameters for the Drude contribution are the scattering rate ($\frac{1}{\tau}$) in cm^{-1} and the dc conductivity in $\Omega^{-1} \text{ cm}^{-1}$. The plasma frequency for the Drude component is calculated automatically by the program. For the Lorentz fit, the parameters include $\Delta\epsilon$ (change in the dielectric constant), the central frequency of the oscillator in cm^{-1} , and the damping in cm^{-1} . The oscillator strength or plasma frequency for the Lorentz fit is also readily calculated. In the case of noisy data such a fit can be used for smoothing the data before the Kramers-Kronig analysis is done.

4.1.5 Smoothing of the Reflectivity Data

The fitted reflectivity data was exported to origin program which was used for smoothing of the experimental reflectivity data. The data was smoothed using the relation;

$$R_{smoothed} = \frac{(R_{experimental} \times 1) + (R_{fitted} \times 2)}{3} \quad (4.5)$$

Where R is the reflectivity. In addition to smoothing with the above equation the noise in the data is removed. Using the smoothed reflectivity data free of noise, Kramers - Kronig analysis is performed and the obtained smooth conductivity is later used for spectral weight calculations and extended Drude analysis.

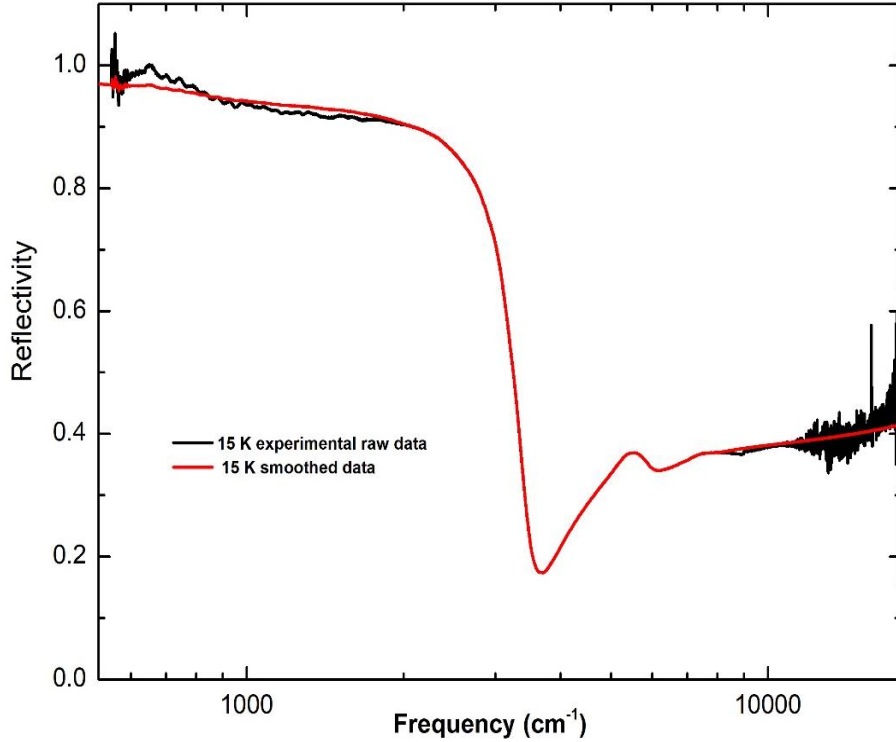


Figure 4.3: smoothed reflectivity spectra of WP_2 compared to unsmoothed reflectivity over a wide range of frequencies for 15 K temperature.

4.1.6 Spectral-weight analysis

The optical constants of solids obey a variety of sum rules whose origins can be traced back to fundamental conservation laws and are intimately connected to the causality principle [92]. Analysis of the sum rules can be used to study the distribution of the spectral weight in correlated electron systems. Of special importance is the sum rule that deals with the integration of the real part of the optical conductivity. The spectral weight is simply this

integrated real-part conductivity as shown in Eq. (2.6). Due to experimental constraints, the integration to infinite frequency in Eq. (2.6) can rarely be done and, therefore, a spectral weight analysis confined to a limited frequency range is used, i.e.:

$$SW(w_c) = \int_0^{w_c} \sigma_1(w) dw = \frac{4\pi n e^2}{m} = w_p^2 \quad (4.6)$$

where w_c is a cut-off frequency. Equation (4.6) is referred to as a partial sum rule. Since the complex conductivity obtained from optical spectroscopy is in units of $\Omega^{-1} \text{ cm}^{-1}$, it has to be converted to units of cm^{-1} , in which case a factor 30 is introduced in Eq. (4.6), while the measured frequency (ν) has to be multiplied with 2π to get w , thereby introducing another factor $\frac{1}{2\pi}$ in Eq. (4.6).

In short, a factor of $\frac{15}{\pi}$ is introduced in Eq. (4.6) and we get:

$$SW(w_c) = \frac{120}{\pi} \int_0^{w_c} \sigma_1(w) dw \quad (4.7)$$

The factor in front of the integral is sometimes written as $\frac{Z_0}{\pi^2}$, where Z_0 is the vacuum impedance ($Z_0 = 377\Omega$). By choosing a reasonable cut-off frequency w_c , so as to consider only the intraband transitions and leaving out the interband transitions at high frequency, the plasma frequency, w_p , can be obtained from which the carrier density is determined.

4.1.7 Extended Drude analysis

The extended Drude analysis is a common tool to obtain insight into low energy excitations and relevant scattering mechanisms of correlated electron system. From this analysis, the scattering rate and normalized effective mass are obtained. It must be emphasized that the units of the optical conductivity must be in cm^{-1} while the measured frequency must be multiplied by 2π for such an analysis. Further details on the extended Drude analysis has already been outlined in Section 2.1.3.

Chapter 5

RESULT PRESENTATION AND DISCUSSION

In this dissertation work the investigated sample was tungsten diphosphide WP_2 , a type II Weyl semimetal with outstanding properties such as extremely large conductivity comparable to pure copper single crystals, extremely long sub-millimeter mean free path comparable to bismuth and extremely large anisotropic MR of 2-3 order magnitude, unique to any Weyl or Dirac semimetal. The results for WP_2 are here presented.

5.1 Resistivity of WP_2

As earlier referred to, resistivity (transport) measurements of WP_2 were performed with an in house University of Stuttgart PI1 (First Physichalisches Insitute) resistivity measurement device. Electrical leads were attached to the sample using the four point probe method. Fig.5.1 shows the resistivity of WP_2 that was obtained as a function of temperature ranging from room temperature to 2 K, with the insert presenting a detailed temperature dependence of the resistivity at low temperatures, that is ($\sim$ below 100 K). Such measurements were compared with those measured at higher currents (20 - 60 mA) and those measured by Kumar etal [86], where it was discovered that applying high currents resulted in overheating, causing some jumps in the measurements. Hence, 5 mA measurements were adopted for the current research. Further, it could be seen that while the results presented here agree very well with those obtained by Kumar etal [86] at low temperatures, at higher temperature there is a huge difference with the resistivity being higher than those of Kumar etal [86] higher temperature.

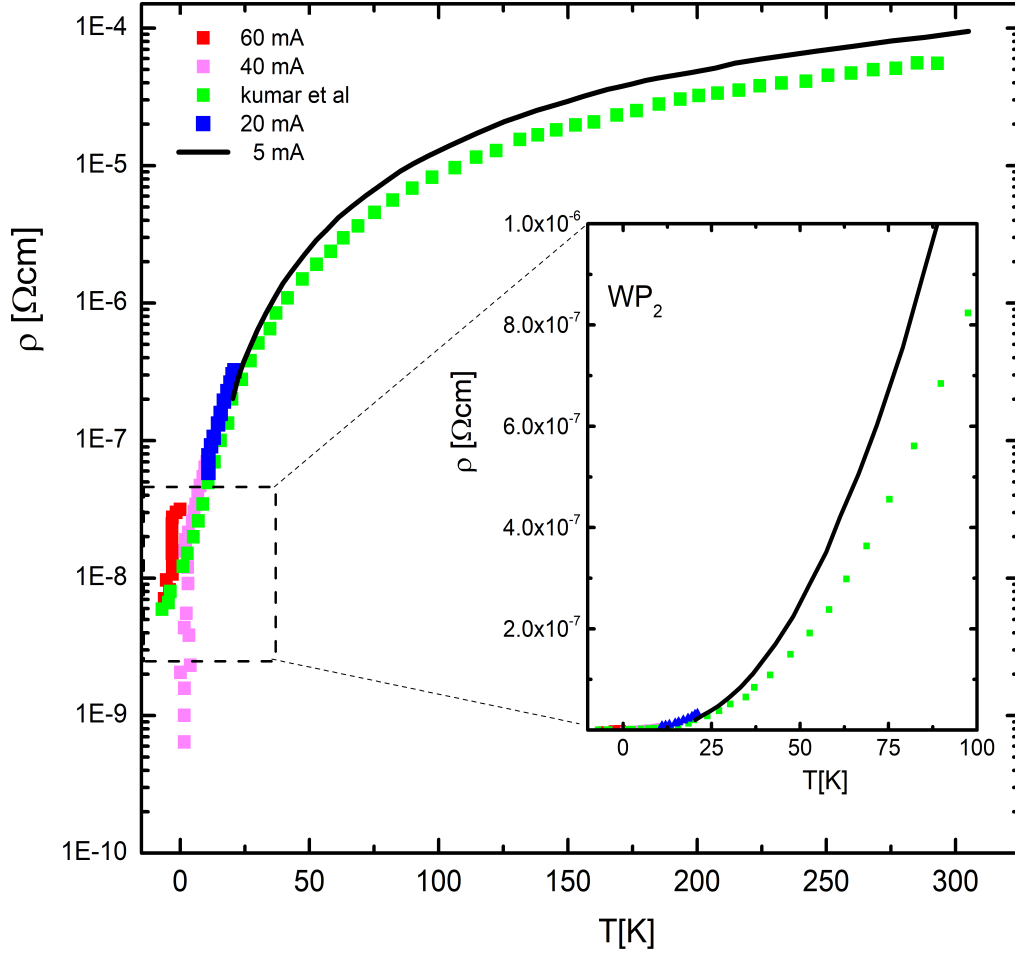


Figure 5.1: Temperature dependence of the in-plane resistivity of WP_2 single crystals. The Inset shows a temperature dependence of the resistivity at low temperatures i.e. $T < 100$ K.

The temperature dependence of the resistivity can be described by the power law;

$$\rho(T) = \rho_0 + AT^n \quad (5.1)$$

with $\rho_0 = 2.57 \times 10^{-7} \Omega\text{cm}$, $A = 1.3 \times 10^{-9} \Omega\text{cmK}^{-2}$ and $n = 2$ from 2 K up to 200 K. To further demonstrate these results, the resistivity data of WP_2 is plotted in Fig. 5.2 as a function of T^2 . From this figure, the quadratic temperature dependence of the resistivity is clearly evident for temperatures below 200 K (i.e., below $40\,000 \text{ K}^2$). This dependence can be accounted for by the usual electron-electron (e-e, T^2 behavior) scattering mechanism, which dominates at low temperatures. This behavior has been observed in other Weyl semimetals

such as TaAs (Tantalum Arsenide) [86], WTe² (Tungsten Ditelluride) [95] and NbP (Niobium Phosphide) Ref. [38]. The quadratic temperature dependence at low temperatures is consistent with the Fermi liquid theory [93, 94]. In weyl semimetals, the T²- dependence is particularly prominent in clean samples where impurity scattering is minimized, emphasizing the role of electron correlations in determining their transport properties [95].

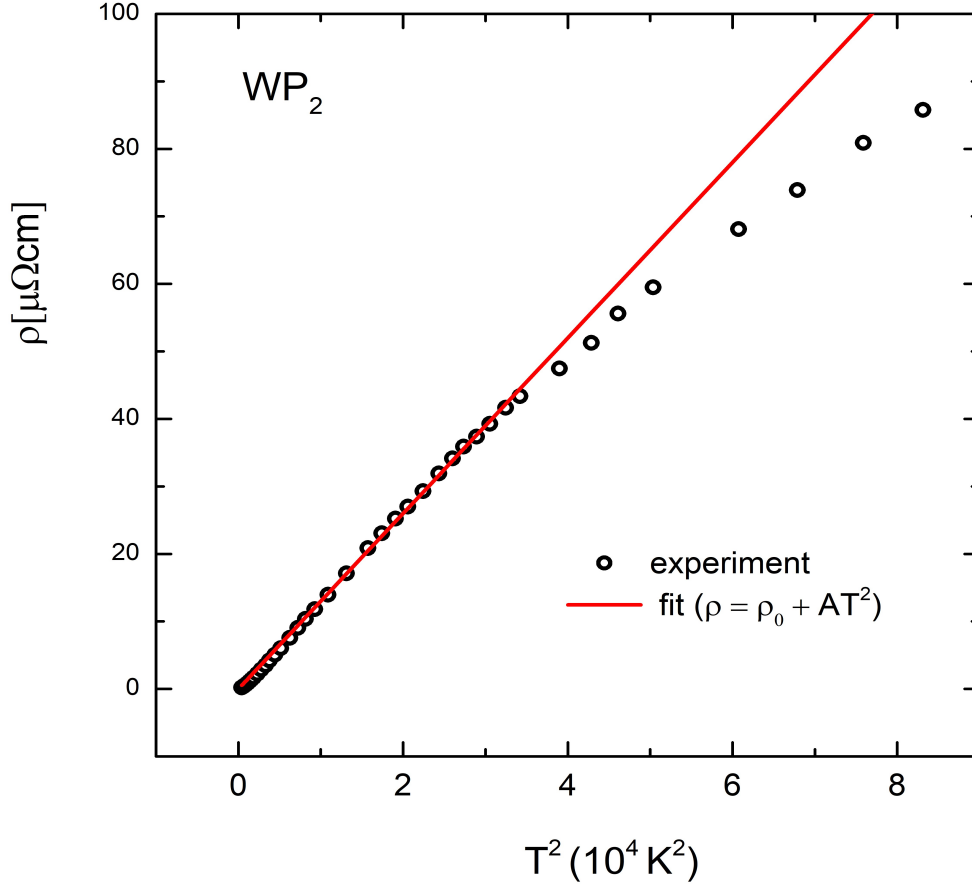


Figure 5.2: : In-plane resistivity as a function of T^2 .

It is observed that as the temperature decreases from 300 K to below 50 K, resistivity (ρ) decreases sharply indicating metallic behavior primarily due to reduction of scattering mechanisms. The topological robustness of WP₂ against scattering also ensures that carriers maintain their momentum over long distances (mean free path), further reducing the resistivity at lower temperatures. Below ~ 10 K, the resistivity saturates and becomes temperature independent, suggesting that residual resistivity dominates. In contrast for, temperatures exceeding 200 K, the resistivity shows a reduced quadratic temperature dependence. This behavior arises from an increase in thermal energy of the charge carriers resulting in more

phonon-electron scattering thereby reducing the mean free path of the charge carriers. To further account for the deviation in the quadratic temperature dependence of the resistivity at higher temperatures ($\sim$ above 200 K) a linear fit was used as shown below in Fig. 5.3.

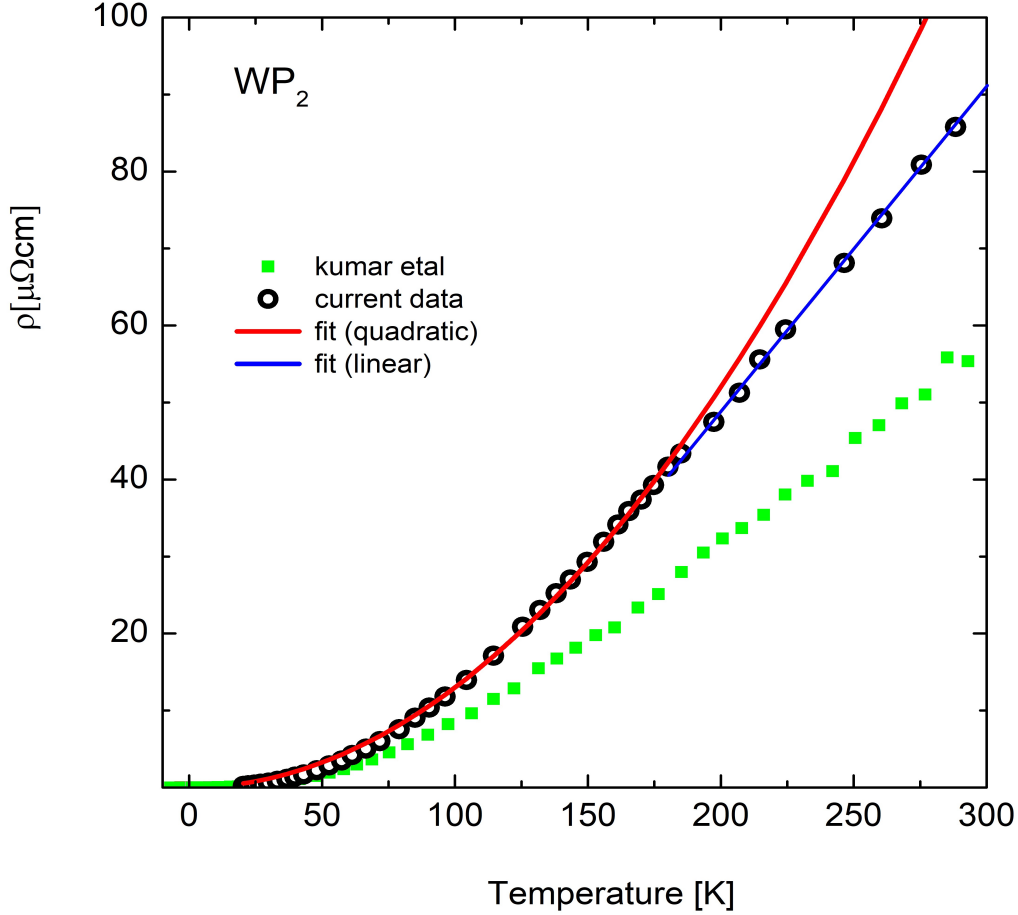


Figure 5.3: In-plane resistivity for the current data compared to data of Kumar etal [86] as a function of Temperature. The red line is a quadratic fit and the blue line is a linear fit

The resistivity (ρ) of WP_2 at higher temperatures ($\sim$ above 200 K) exhibits a linear temperature dependence which is indicative of dominant electron-phonon scattering. The smallest resistivity value observed at 2 K was $\rho \sim 2 \times 10^{-8} \Omega\text{cm}$ while that at 300 K was $\rho \sim 9.5 \times 10^{-5} \Omega\text{cm}$ yielding extremely large residual resistivity ratio ($\text{RRR} = \rho(300 \text{ K}) / \rho(2 \text{ K})$) of $\text{RRR} \approx 47,000$. To the best of my knowledge, this very high value of RRR is the largest so far reported in any binary compound. MoP_2 with a similar structure also shows a similar temperature dependence of resistivity with $\text{RRR} \approx 2578$ [86]. While this may be an indication

of a very high purity of the WP_2 crystals studied here, another more intriguing possibility is that the unique electronic properties of these compounds make certain scattering mechanisms less likely through topological protection. As a result of all these factors WP_2 has an extremely large conductivity and high magnetoresistance as earlier stated.

5.2 Reflectivity of WP_2

In this dissertation optical reflectance measurements of the single crystals of WP_2 with the electric field (E) and the incident light applied along its crystalline c-axis and a-axis plane with frequencies ranging from 540 cm^{-1} - $20\,000 \text{ cm}^{-1}$ at various temperatures ranging from 15 K-300 K was measured and is shown Fig. 5.4 below. The insert in both shows the lower frequency region of the reflectivity at various temperatures.

The reflectivity spectral as a function of temperature at lower frequencies seem to approach absolute reflectance (i.e. $R = 1$) at zero frequency and varies approximately linearly with frequency. At lower frequencies i.e. below 1000 cm^{-1} for both spectra as seen from the insert in Fig. 5.4 (a) and (b) respectively, the reflectivity increases with a decrease in temperature typical for metals. As the frequency increases from 1000 cm^{-1} - 4000 cm^{-1} , the reflectivity gradually decreases i.e. for instance the lowest measured temperature 15 K in both spectra, the reflectivity drops quite sharply between 1000 cm^{-1} to 4000 cm^{-1} from ~ 0.94 to ~ 0.18 for E //c -axis plane and ~ 0.95 to ~ 0.22 for E//a - axis plane respectively then forms a plasma peak like feature around 4000 cm^{-1} which is indicated by the black arrow as shown in Fig. 5.4 (a) and (b) respectively confirming a good metallic behavior.

Above 4000 cm^{-1} , an upturn in the reflectivity is evident in both spectra, where there is a different temperature dependence from that at lower frequencies i.e. increase in temperature results in increase in the reflectivity especially between the frequency range 4000 cm^{-1} to 6500 cm^{-1} . However, besides the usual Drude response, one other distinct feature observed in the reflectivity spectra which becomes particularly prominent is an anomaly or crossing points in both spectra i.e. at higher frequencies i.e. of $\sim 10\,300 \text{ cm}^{-1}$ for E//c and $\sim 9000 \text{ cm}^{-1}$ E//a as shown under a dotted square in Fig 5.5 (a) and (b) respectively. The overall reflectivity changes behavior at these crossing points i.e. reflectivity increases with increase in temperature especially at higher frequencies due to redistribution of the spectral weight of the charge carriers (holes and electrons) from low frequencies to high frequencies on heating.

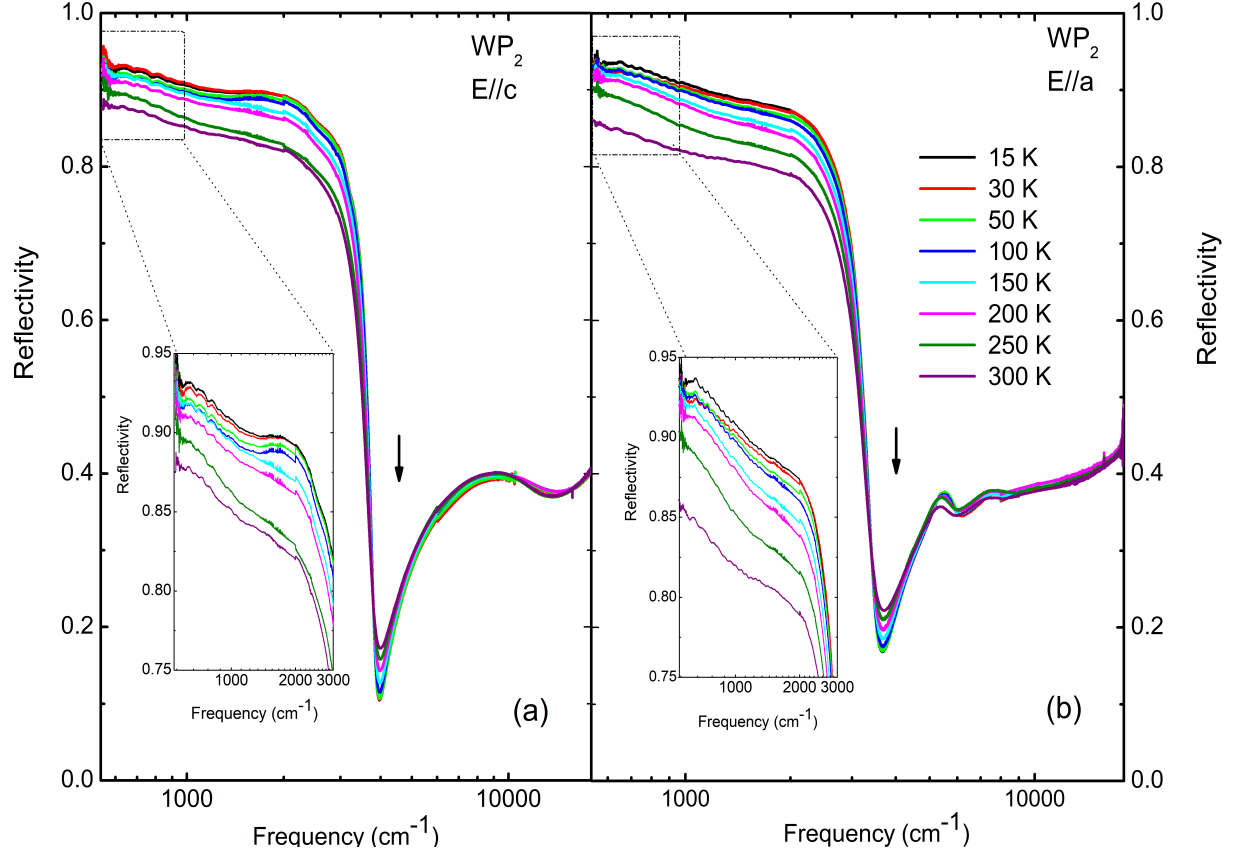


Figure 5.4: (a) and (b) Reflectivity of WP_2 measured using FTIR spectroscopy at different temperatures for $E//c$ and $E//a$, respectively. (Inset) Expanded plots showing the low-frequency regime.

For all the measured frequencies, the hump-like features at intermediate frequencies i.e. around $10\,000\text{ cm}^{-1}$ in Fig 5.5 (a) and between 5500 cm^{-1} to $8\,000\text{ cm}^{-1}$ in Fig 5.5 (b) signals the presence of several interband transitions and exhibit a strong temperature dependence at such frequencies. It should be noted that the reflectivity increase is much stronger at lower frequencies compared to higher frequencies. With decreasing temperature, the overall reflectivity increases at lower frequencies while at higher frequencies increase in temperature tends to increase the reflectivity, indicating an increasing metallicity as it is expected for semi metallic compounds with reflectivity as a function temperature.

Figure 5.6. shows a well-defined sharp reflectance edge at 300 K emerging in these spectra, followed by a reflectance valley denoted as $V_a \sim 3700\text{ cm}^{-1}$ for $E//a$ axis plane and $V_c \sim 4000\text{ cm}^{-1}$ for $E//c$ axis plane. The edges are relatively sharp and shifts to higher frequencies with increasing temperature indicating a temperature dependent direct energy bandgap of around $0.3\text{ eV} - 0.4\text{ eV}$. This energy range of the plasma edge is much higher than that of typical

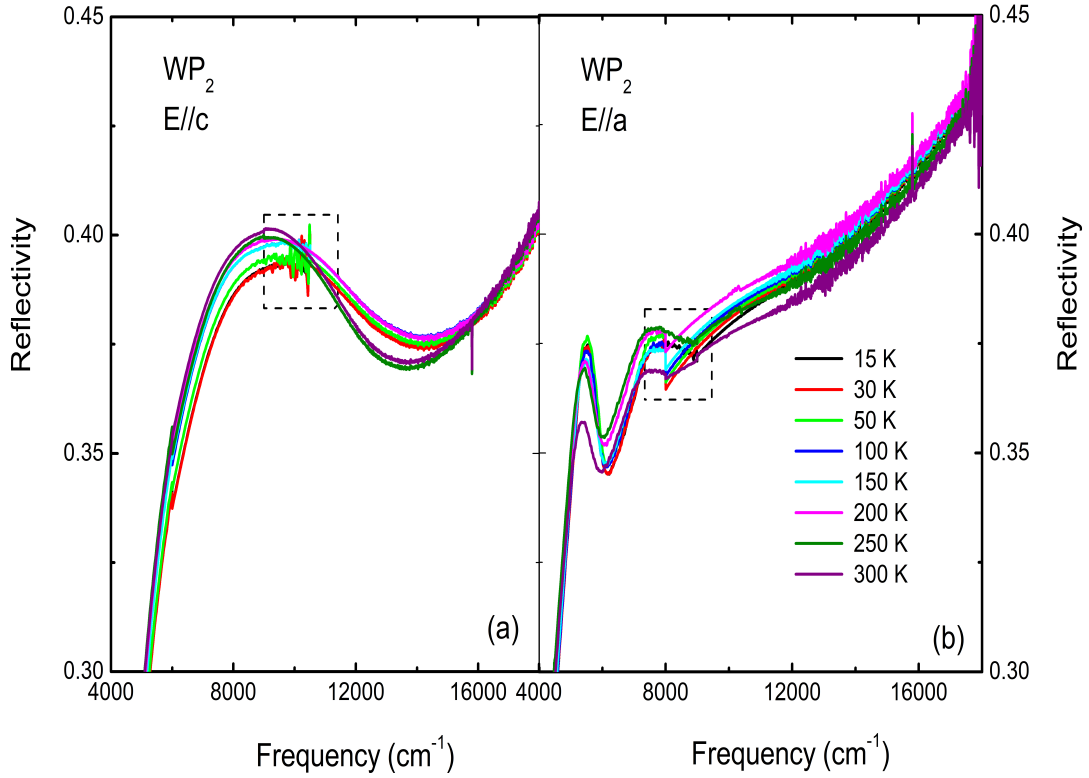


Figure 5.5: reflectivity of (a) $E // c$ - axis plane and (b) $E // a$ - axis plane showing the crossing points (the area under the dotted square) and hump like features at higher frequencies.

semimetals investigated previously (e.g., < 0.08 eV for bismuth [93,94] and WTe_2 [95, 96]). A reflectance valley typically develops near the screened plasma frequency. Therefore, variation in wave numbers for $E // a$ and $E // c$ valley reflect anisotropy in the plasma frequency of the sample [97]. The valley wave number ratio V_c/V_a is (~ 1.2), consistent with what Zhang et al obtained when they did similar calculations of the quantitative analysis of the plasma frequency of $E // a$ and $E // c$ by using the RefFIT program i.e. $w_{p,c}/w_{p,a}$ was (~ 1.3). Anisotropy is the directional dependence of a material's physical properties. This means that the properties of a material, such as electrical conductivity or optical response, vary when measured along different crystallographic directions this can have significant application in optoelectronics and thermoelectric applications [98] .

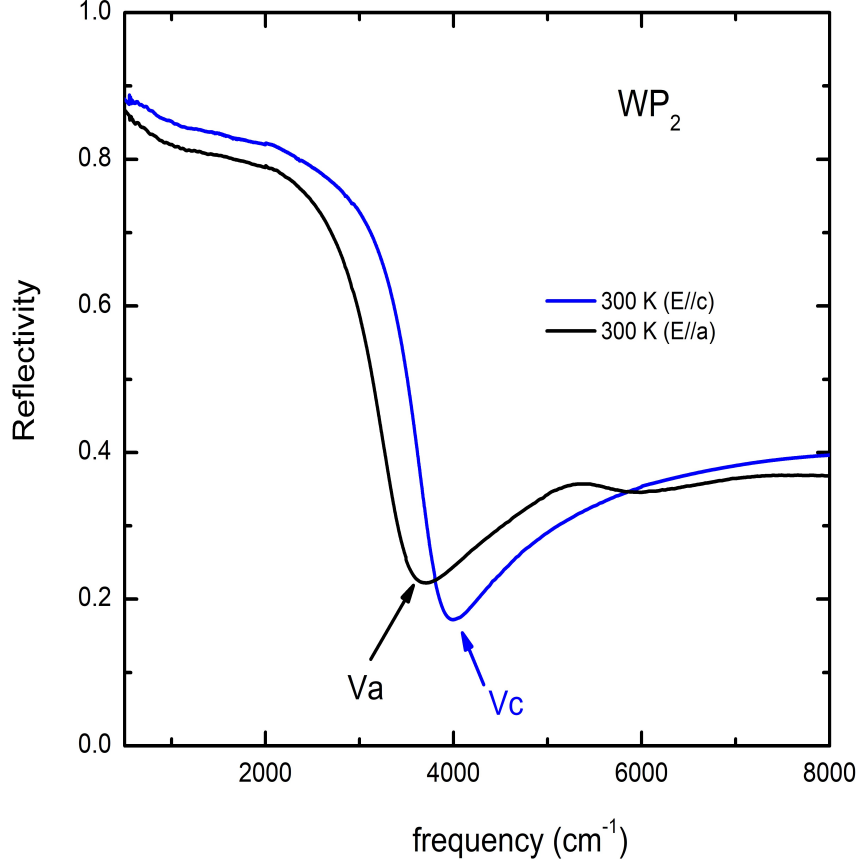


Figure 5.6: Anisotropic reflectance of WP_2 shown by the valleys denoted as V_a and V_c , respectively.

5.3 Conductivity of WP_2

Figure 5.7 shows the real and imaginary parts of the complex optical conductivity of WP_2 for $E//c$ and $E//a$ plane axis respectively calculated through Kramers-Kronig analysis over a wide range of frequencies at various temperatures. The real part of the optical conductivity (σ_1), as plotted in Fig 5.7 (a) and (b), allows for a more detailed view on the optical properties of WP_2 as a function of temperature. At lower frequencies, the real part of the optical conductivity (σ_1) shows a temperature dependent behavior at i.e. for frequencies below 1000 cm^{-1} in both spectra, σ_1 shows a temperature-dependent behavior dominated by the Drude-like free-carrier response. At low temperatures (15 K – 30 K), the real part of the optical conductivity is higher due to reduced electron-phonon scattering and enhanced carrier mobility. As temperature increases (200 K - 300 K), the real part of the optical conductivity decreases significantly due to electron-phonon interactions thereby reducing carrier mobility. As the frequency increases from 1000 cm^{-1} to 4000 cm^{-1} , the real part of the op-

tical conductivity (σ_1) for both spectra decreases for all measured temperatures. However, above 4000 cm^{-1} an upturn is observed in both spectra where the real part of the optical conductivity increases almost linearly up to a maximum close to $10\,000 \text{ cm}^{-1}$ in Fig. 5.7 (a). And as for Fig. 5.7 (b) the real part of the optical conductivity above 7000 cm^{-1} increases almost linearly as well up to the highest measured frequency ($20\,000 \text{ cm}^{-1}$).

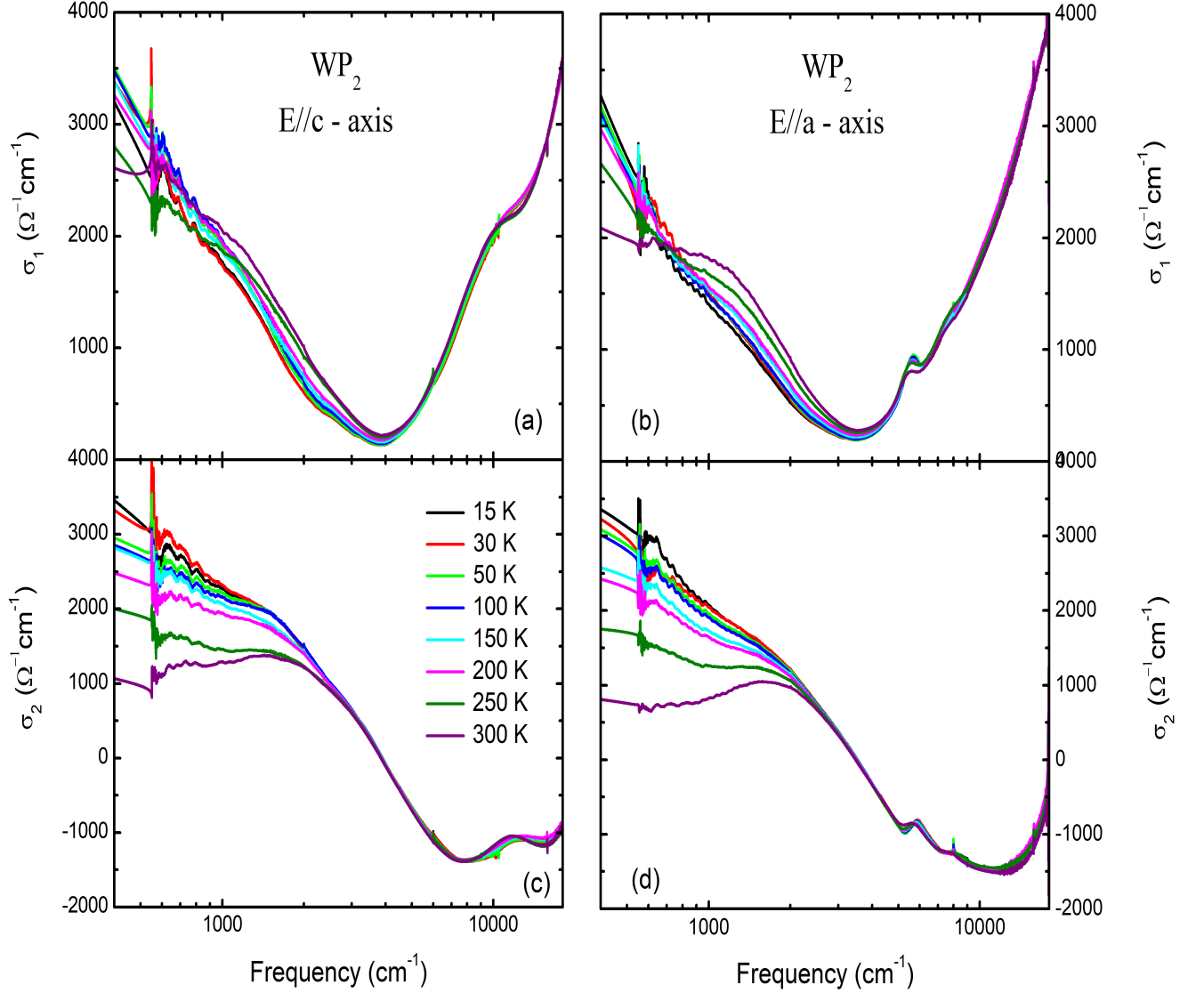


Figure 5.7: Frequency dependence of the real part and imaginary part of the optical conductivity for WP_2 at various temperatures.

The real part of the optical conductivity for both spectra shows that various temperatures cross each other at both the lower and higher frequency range i.e. around 1000 cm^{-1} and $10\,000 \text{ cm}^{-1}$ in Fig. 5.7 (a) as well as around 1000 cm^{-1} and 6000 cm^{-1} in Fig. 5.7 (b) respectively. This behavior is a clear signature of spectral-weight transfer from the mid-infrared regime to low frequencies on cooling, leading to Drude-like contributions at low frequencies narrowing and sharpening on cooling. The hump like feature in Fig. 5.4 (a) around 5000 cm^{-1} can be attributed to interband transitions. The imaginary parts of the complex optical conductivity thus obtained for WP_2 are shown in figure 5.7 (c) for $E // c$ and 5.7 (d) for $E // a$ respectively. At lower frequencies in both spectra i.e. below 3000 cm^{-1} the imaginary part of the optical conductivity $\sigma_2(\omega)$, increases with decreasing temperature. From theory $\sigma_2(\omega)$, has to increase with frequency passing through a maximum before starting to decrease with further increase in frequency. The frequency corresponding to the maximum is ascribed to $\frac{1}{\tau}$ of the sample. However, no clear maximum in $\sigma_2(\omega)$, implying that $\frac{1}{\tau}$ for this WP_2 is below the measured frequency range.

Beyond 3000 cm^{-1} the imaginary part of the optical conductivity $\sigma_2(\omega)$, monotonically decreases to zero and becomes negative above 4000 cm^{-1} in both spectra signaling of onset interband transitions above such frequencies. At higher frequencies i.e. $\sim$ around $10\,000 \text{ cm}^{-1}$ there is a hump like feature in Fig. 5.7 (c) and a valley like feature in Fig. 5.7 (d) around the same frequency range in which can be attributed to interband transitions.

It is notable from Fig. 5.8 (a) and (b) that there is a linearity behavior observed in the overall optical conductivity of WP_2 , in the MIR and NIR region for both spectra is due to the unique electronic structure of WP_2 specifically from the linear energy dispersion near the Weyl points. This similar behavior has been observed in other Weyl semimetals such as TaAs [99], MoTe_2 and WTe_2 [100]. Zukova et al also observed linearity when they did similar studies on $\text{Bi}_2\text{Te}_2\text{Se}$, and attributed linearity to complex interactions between multiple bands and not the 3D Dirac bands [101]. Weyl semimetals host quasiparticles called Weyl fermions, which arise due to splitting of the degenerate Dirac points in momentum space. Near the Weyl points, the energy dispersion is linear meaning the energy E is proportional to the momentum K i.e. $E \propto K$. It's this linear dispersion that may lead to unique optical properties.

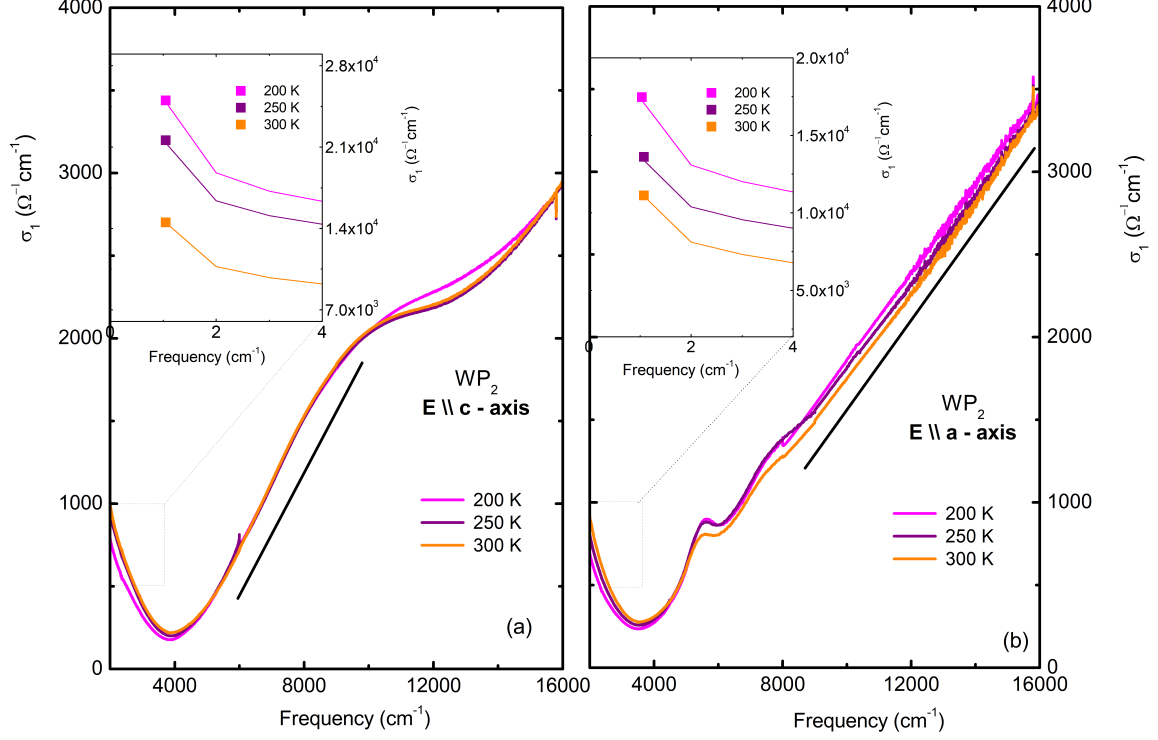


Figure 5.8: The real part of the optical conductivity of WP_2 for $E // c$ (a) and $E // a$ (b). the solid black lines represent linearity in the measured frequency regimes respectively. The markers at less than 2 cm^{-1} in the insert of (a) and (b) represents the dc conductivity calculated from direct current resistivity data [Fig. 5.1].

5.4 Decomposition of the real part of the optical conductivity of WP_2 for $E//c$ axis plane.

To get a feel of the various contributions to the optical conductivity, the real part of the optical conductivity was modeled for 15 K and 300 K for the $E//c$ plane axis orientation using the Drude-Lorentz complex conductivity model:

$$\begin{aligned} \hat{\sigma}(w) &\equiv \sigma_1(w) + i\sigma_2(w) \\ &= \frac{1}{4\pi} \left[\frac{w_p^2 D^\tau}{1 - iw\tau} + \sum_k \frac{w_{pk}^2 w}{\gamma_k w + i(w_{0k}^2 - w^2)} \right] \end{aligned} \quad (5.2)$$

The first term in Eq. (5.2) corresponds to a free-carrier Drude response, characterized by a plasma frequency w_{pD} and a scattering rate τ^{-1} . The second term is a sum of Lorentz oscillators; each of them is characterized by a resonance frequency w_{0k} , a linewidth γ_k , and a plasma frequency w_{pk} . The complex conductivity fit together with its components for WP₂ obtained from this model for 15 K and 300 K is shown in Fig.5.9

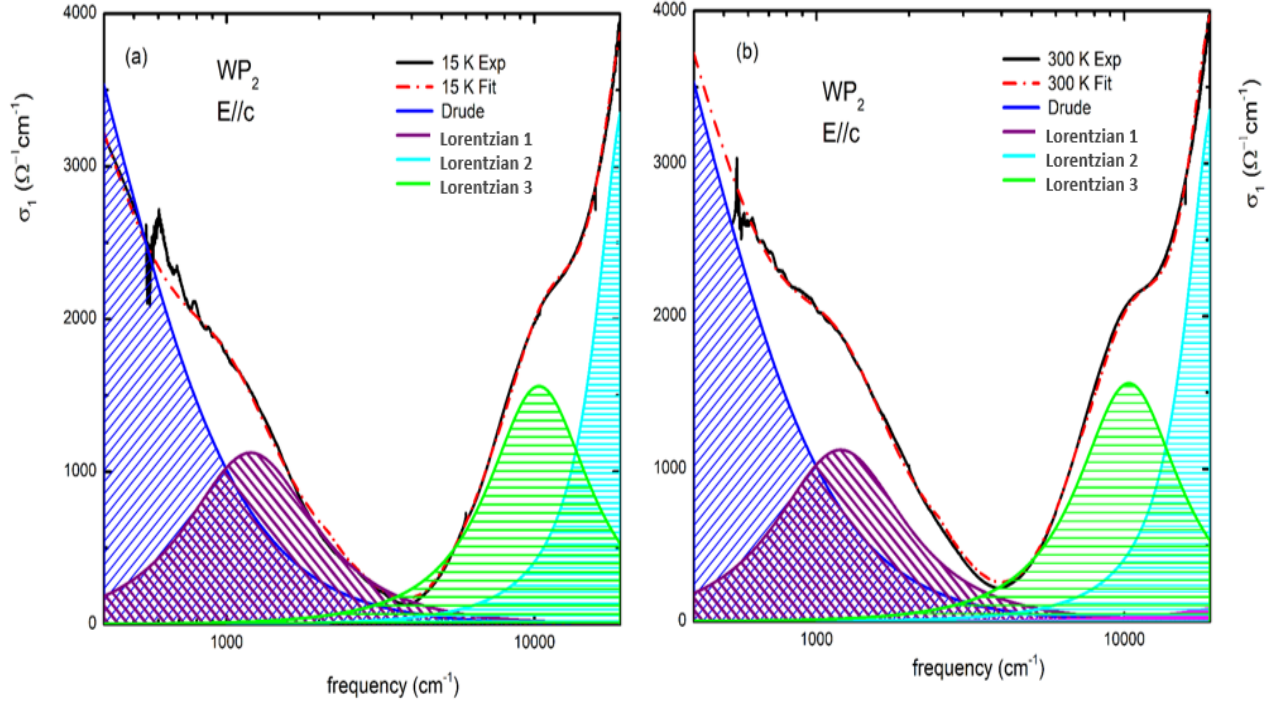


Figure 5.9: Decomposition of the real part of the optical conductivity at 15 K and 300 K for E//c plane axis for WP₂.

It is evident from Fig.5.9 that the real part of the optical conductivity can be decomposed into the Drude contribution and multiple Lorentz oscillators. The Drude contribution dominates at low frequencies, i.e. $> 1000 \text{ cm}^{-1}$ in both the 15 K and 300 K spectra. At 15 K, the Drude peak is narrower, indicating a lower scattering rate (γ) and extremely high mobility of carriers, which is due to the suppression of backscattering that is linked to the topological protection of the Weyl nodes and low scattering rates at low temperatures. For rising temperature up to 300 K, the Drude peak starts to broaden, which indicates increased carrier scattering due to electron phonon interactions and thermal disorder. It should be notable that the Drude component reflects the metallic free carrier behavior, with strong temperature dependence.

The Lorentzian contributions appearing at higher frequencies correspond to interband transitions either near the Weyl nodes or between trivial bands. Lorentz oscillator 1 with a peak at about 1200 cm^{-1} represents low energy intraband transitions, which are sharper and more defined at low temperatures due to reduced thermal broadening. Lorentz oscillator 1 increases with increase in temperature i.e. it grows at the expense of drude peak as temperature increase from 15 K to 300 K. Lorentzian 2 and 3, at higher frequencies highlight transitions involving deeper energy bands. The Lorentzian peaks remain temperature-dependent in position, as they are determined by the band structure, but their broadening and intensity vary with temperature. At 300 K, phonon scattering leads to broader linewidths γ_k , and reduced peak intensities compared to the sharper features observed at 15 K. Across all frequencies, the combined contributions of the Drude and Lorentzian terms define the total optical conductivity.

The behavior observed underscores the metallic nature of WP_2 and the interplay between free carriers and interband transitions, with the Drude term reflecting temperature-sensitive carrier dynamics and the Lorentz contributions providing insight into band structure transitions. This decomposition helps understand the interplay between free carriers and band transitions in WP_2 , making it an invaluable approach for understanding the interplay of scattering mechanisms and electronic structure in complex materials.

5.5 Decomposition of the real part of the optical conductivity of WP_2 for $\mathbf{E} \parallel \mathbf{a}$ -axis plane.

The decomposition of the optical conductivity for WP_2 , analyzed using the Drude-Lorentz model, reveals significant insights into its anisotropic electronic and optical properties. For the $\mathbf{E} \parallel \mathbf{a}$ -axis orientation, the experimental data at 15 K demonstrates a dominant Drude response, evident in the broad and prominent low-frequency peak, which reflects the high mobility of free carriers with minimal scattering. This is consistent with the smaller effective mass that was found along the $\mathbf{a}$ -axis ($m_a^* = 0.8m_o$), allowing electrons to move more freely compared to the $\mathbf{c}$ -axis ($m_c^* = 1.2m_o$). At 300 K, the Drude contribution diminishes due to increased electron-phonon scattering, resulting in reduced carrier mobility. The Lorentzian components, representing interband transitions or localized resonances, remain robust across temperatures, suggesting that these processes are largely temperature-independent. Notably,

five Lorentzian peaks are identified for $E // a$, indicating rich interband transitions that contribute significantly to high-frequency conductivity.

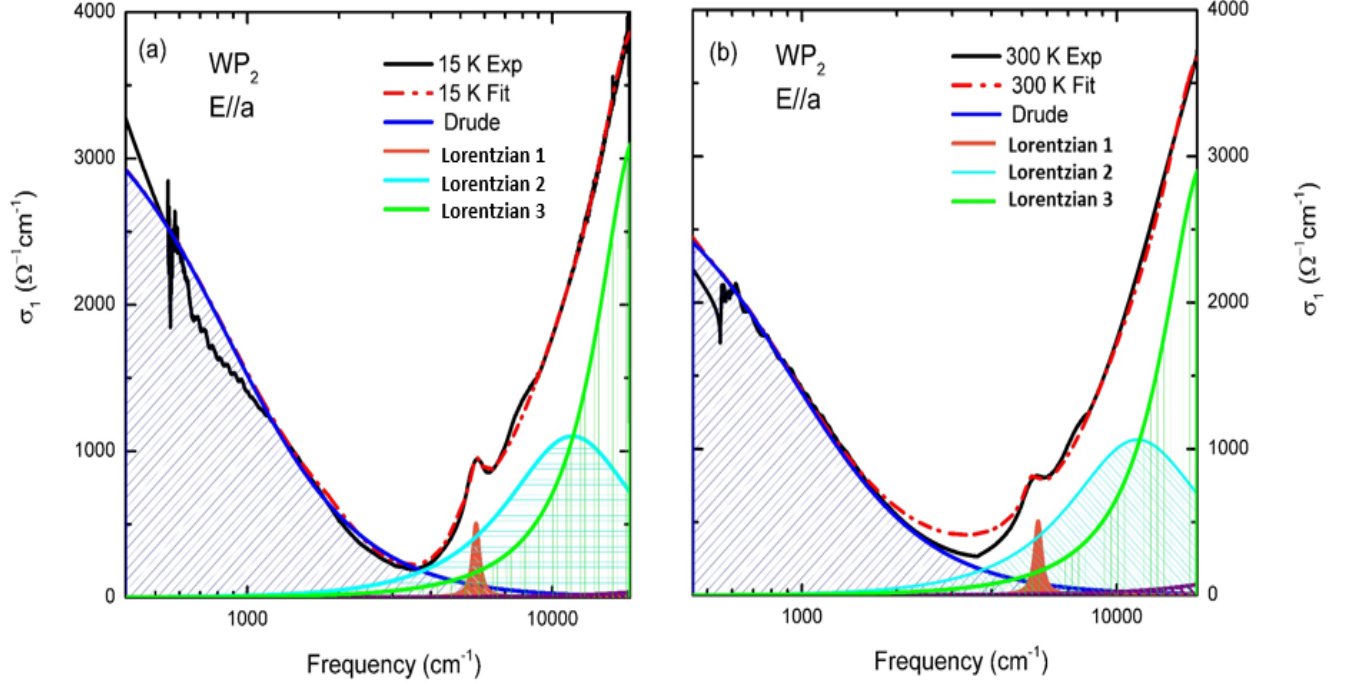


Figure 5.10: Decomposition of the real part of the optical conductivity at 15 K and 300 K for $E//a$ plane axis for WP_2 .

The $E // c$ -axis orientation, the Drude response at 15 K is less pronounced, with a narrower peak compared to $E // a$, reflecting lower carrier mobility due to the heavier effective mass in this direction. At 300 K, the Drude conductivity further decreases as phonon scattering intensifies. Interestingly, the Lorentzian peaks for $E // c$ are fewer (three components) but sharper, highlighting the anisotropic nature of interband transitions in WP_2 . While the Lorentzian terms are temperature-independent for both orientations, their distinct spectral features underscore the optical anisotropy of the material.

Comparing the two orientations, WP_2 exhibits superior conductivity and mobility along the a -axis, supported by the stronger Drude response and a richer spectrum of interband transitions. The c -axis, while less conductive, displays sharper Lorentzian peaks, suggesting directionally dependent optical properties. This anisotropy is a nature of WP_2 's unique electronic structure, which balances free carrier dynamics and robust interband transitions. The reduced conductivity at 300 K for both orientations highlights the role of electron-phonon

interactions, although WP₂'s topological protection and intrinsic properties allow it to retain high performance relative to conventional materials. Together, this analysis illustrates WP₂'s potential for high-mobility electronic applications and its suitability for optoelectronic devices, where directional transport and optical properties can be leveraged effectively.

5.6 Spectral Weight Analysis

In order to obtain a qualitative picture of how the spectral weight in WP₂ is redistributed with temperature, in Fig. 5.11 the total spectral weight, i.e., the integrated real part of the complex conductivity for WP₂ for both E//c and E//a has been plotted.

$$SW(w_c) = 8 \int_0^{w_c} \sigma_1 dw \quad (5.3)$$

In the low-frequency region (below 1000 cm⁻¹), the spectral weight (SW) steadily increases with frequency, indicating the accumulation of electronic contributions to the optical conductivity. This behavior is due to free carriers undergoing intraband transitions, which can be described by the Drude model. At lower temperatures, such as 15 K and 30 K, the SW in this region is noticeably higher compared to higher temperatures like 200 K and 300 K. This increase can be attributed to reduced scattering of charge carriers at low temperatures, as phonon activity and other scattering mechanisms are suppressed. Overall, this temperature-dependent trend signals the metallic properties of WP₂, showing how reduced scattering at low temperatures enhances carrier mobility and optical conductivity.

For all measured temperatures in both curves, the spectral weight increases monotonically with frequency and shows an upturn around 4000-5000 cm⁻¹ which is of importance as it is an indication of spectral weight redistribution starting within this frequency regime. This upturn is due to the interband transitions, which dominate the optical spectra at such frequencies. The upturn also shows evidence of a plasma edge observed in both plane axes as previously referred to. Up to 10,000 cm⁻¹ the spectral weight still shows minimal temperature dependence and it is only at higher frequencies above 10,000 cm⁻¹ where the spectral weight does not show temperature dependence and all the curves seem to converge at ~ 10 000 cm⁻¹, implying that the spectral weight is only conserved beyond 10,000 cm⁻¹, which is maybe a clear indication of correlation effects in this material. In other correlated electron materials, the spectral weight is known to be conserved also only at frequency scales of a few

electron volts (eV) [102, 103, 104]. Thus, the conservation of spectral weight observed only beyond $10,000 \text{ cm}^{-1}$ might be an indication of the presence of electron correlations in WP_2 .

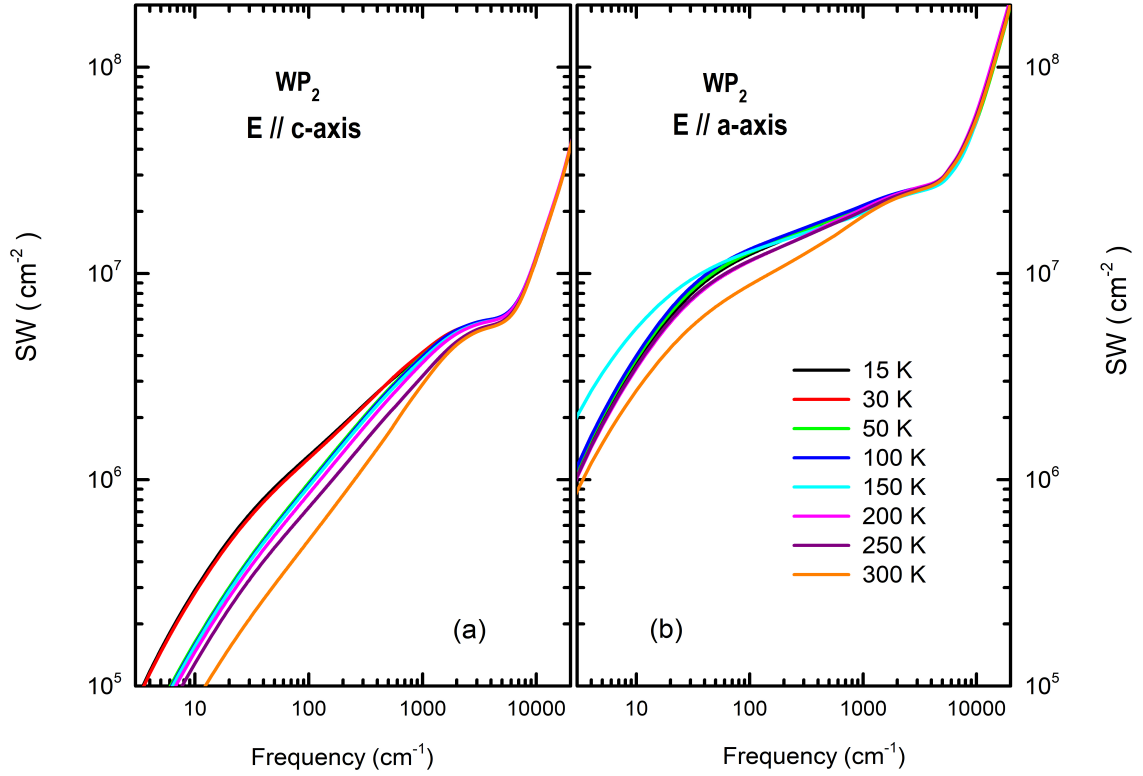


Figure 5.11: Frequency dependence of the spectral weight of WP_2 for E // c and E // a at various temperatures indicated.

From the normalized spectral weight, it can be clearly seen that as the temperature increases, the loss in spectral weight becomes minimal. The purpose of the normalized spectral weight is to identify the cut-off frequency which is chosen as a minimum from the lowest temperature curve to calculate the plasma frequency. For the lowest temperature curve has to be chosen From Fig. 5.11. It is clear that at low frequencies (below $\sim 8000 \text{ cm}^{-1}$ all the spectral weight curves are above the dashed red line (300 K), indicating that the spectral weight at lower temperatures, i.e., 15 K and 30 K, is higher than at 300 K. On cooling from 300 K to 15 K at lower frequencies, accumulation of spectral weight is observed and it is compensated for in the range 9000 cm^{-1} to $20,000 \text{ cm}^{-1}$ leading to $\frac{SW(T)}{SW(300K)} < 1$. However, the ratio, i.e. $(\frac{SW(T)}{SW(300K)})$ goes through a minimum at $\sim 10,800 \text{ cm}^{-1}$ for low temperatures, i.e. 15 K and 30 K.

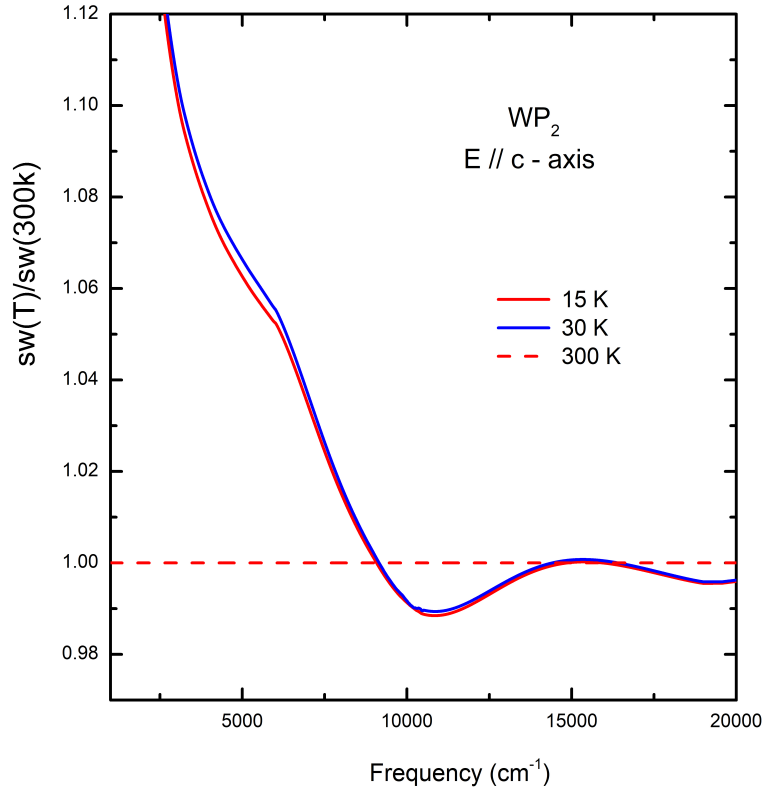


Figure 5.12: Variation of the normalized spectral weight for WP_2 over a wide range of frequencies and at 15 K and 30 K.

In order to estimate the plasma frequency of the itinerant charge carriers only, the frequency corresponding to the minimum in the normalized spectral weight was chosen to be the cut-off frequency (w_c) i.e. $10\,800\text{ cm}^{-1}$, thus cutting off the contributions from interband transitions. From such an analysis, a plasma frequency ($w_p/2\pi$) of $\sim 7965\text{ cm}^{-1}$ for both plane axes was obtained for WP₂. Using the relation between the charge-carrier density, n , and the plasma frequency (w_p), i.e., $\frac{4\pi ne^2}{m} = w_p^2$, $n = 2.5 \times 10^{21}\text{ cm}^{-3}$ was estimated for WP₂, by assuming m to be equal to the free-electron mass, m_o . This charge carrier density of WP₂ calculated here is slightly higher than in other wely semimetals i.e in certain Nb- and Ta-based compounds, the charge carrier density lies between 10^{18} and 10^{20} cm^{-3} . [105]

5.7 Extended Drude Analysis.

To get an insight into the effect of many-body interactions on the itinerant behavior of charge carriers in WP₂, an extended Drude analysis was performed. From such an analysis, the optical scattering rate ($\frac{1}{\tau}$) and the effective mass ($\frac{m^*}{m}$) for E // c and E // a axes as shown in Fig. 5.13. (a) and (b) respectively, were obtained using a plasma frequency of 7965 cm^{-1} (see spectral weight analysis above).

From Fig. 5.13. (a) and (b) It is evident that the scattering rate at low frequencies i.e. $\sim$ below 2000 cm^{-1} for both orientations increases with increasing temperature, a clear indication of stronger electron-phonon scattering at higher temperatures, which is typical for metallic systems. The low frequency region i.e. that is the insert Fig. 5.13. (a) and (b) for both spectra shows that the scattering rate increases monotonically with temperature up to about 4000 cm^{-1} which corresponds to the point where there is maximum increase in the scattering rate.

Beyond 4000 cm^{-1} the scattering rate decreases monotonically and exhibit no saturation for both spectra which implies that the scattering mechanism becomes less dependent on frequency, and more likely due to the dominance of intrinsic electronic properties over extrinsic scattering mechanisms. Around 4000 cm^{-1} the scattering rate shows a peak in both curves that is consistent across all temperatures, which could be attributed to interband transitions at such frequencies. Additionally, the normalized effective mass as shown in Fig. 5.13. (c) and (d) is analyzed in relation to frequency across temperatures ranging from 15 K to 300 K. At low frequencies i.e. below 2000 cm^{-1} the effective mass is relatively constant in both curves with values shifting from 0.2 to 0.8 in Fig. 5.13. (c) and from 0.7 to 1.2 in Fig. 5.13.(d), indicating minimal renormalization of the effective mass. However, at higher

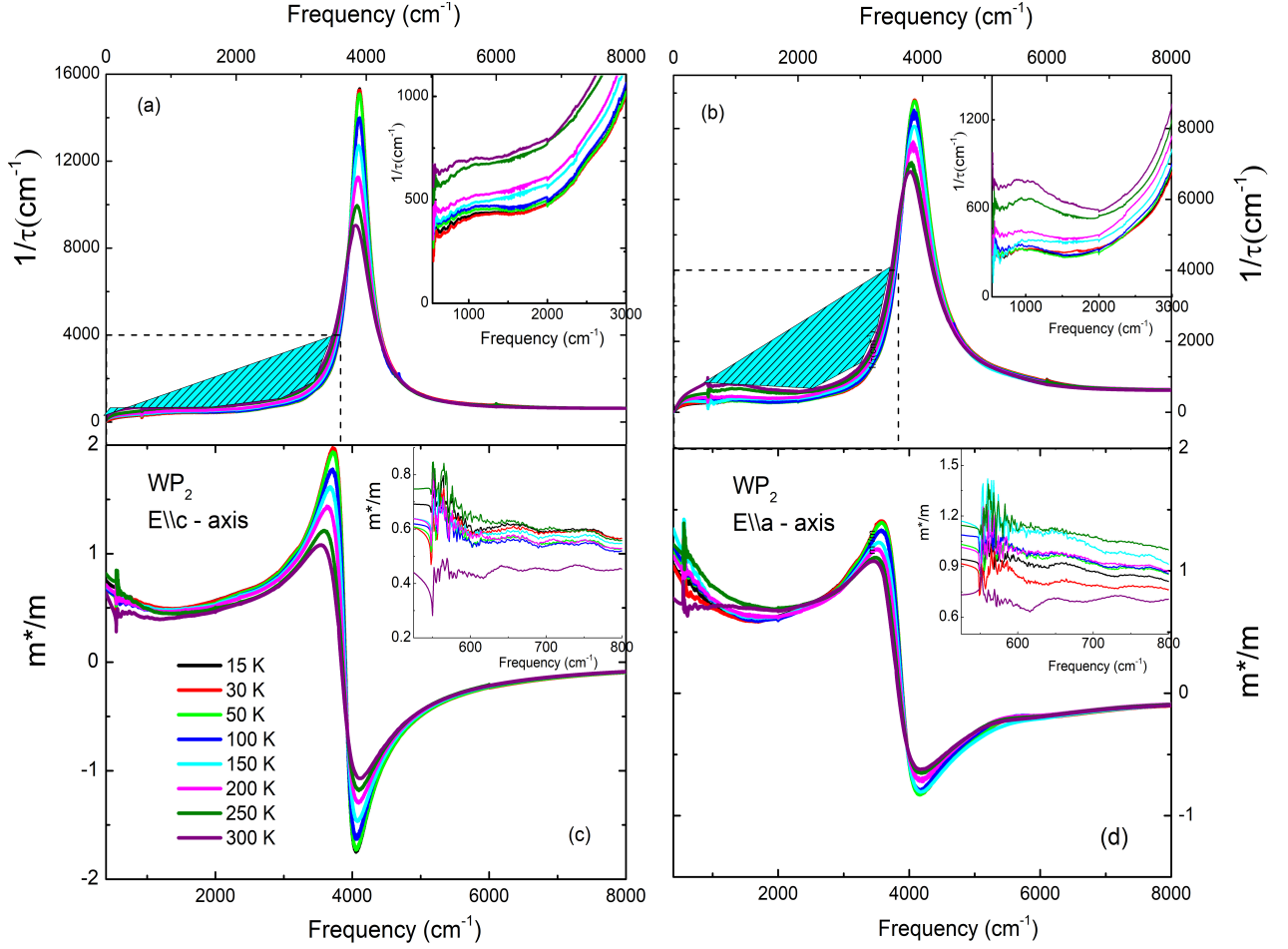


Figure 5.13: ((a) and (b) Frequency dependence of scattering rate (τ^{-1}) for $\text{E} \parallel \text{c}$ and $\text{E} \parallel \text{a}$ respectively, with insert showing the low frequency region i.e. frequencies below 3000 cm^{-1}). The light cyan shaded area presents the Landau-Fermi-liquid (LFL) regime, a regime where quasiparticles are supposed to be well defined. (c) and (d) Mass enhancement factor ($\frac{m^*}{m}$) for $\text{E} \parallel \text{c}$ and $\text{E} \parallel \text{a}$ axis plane respectively, with insert showing the low frequency regime i.e. frequencies below 1000 cm^{-1}).

frequencies for both spectra, a significant dip occurs around 4000 cm^{-1} , which corresponds with a peak in the scattering rate ($\frac{1}{\tau}$) and its temperature dependent i.e. it becomes more pronounced at higher temperatures. This behavior implies a strong interaction between electronic states and phonons or interband transitions at such frequencies. It is notable that both orientations exhibit saturation in the effective mass at higher frequencies (beyond 4000 cm^{-1}). This saturation indicates that the effective mass becomes independent of frequency, reflecting the intrinsic band structure of WP_2 .

5.8 Dielectric constant for WP₂

The optical dielectric function of WP₂ was investigated for both orientations, $E \parallel a$ axis and $E \parallel c$ axis. The real (ϵ_1) and imaginary (ϵ_2) parts of the dielectric constant as functions of frequency are shown in Fig. 5.15. The real part, ϵ_1 for both orientations, exhibits large negative values at low frequencies i.e. below 2000 cm⁻¹, indicative of metallic behavior, where free carrier screening dominates. As the frequency increases above 2000 cm⁻¹, ϵ_1 increases monotonically and transitions toward zero becoming slightly positive and constant for all temperatures in both orientation, this reflects a transition from metallic to dielectric like behavior. This behavior is more pronounced at lower temperatures, where ϵ_1 is significantly more negative in the low frequency regime i.e. below 2000 cm⁻¹, consistent with a higher density of free carriers and reduced scattering. Conversely, at higher temperatures, ϵ_1 becomes less negative due to increased carrier scattering, as predicted by the Drude model.

Similarly, the imaginary part, ϵ_2 , in Fig. 5.15. (c) and (d) exhibits large values at low frequencies, signifying energy dissipation from free carrier dynamics, which diminishes as the frequency increases and the material becomes more transparent. At lower temperatures, ϵ_2 is higher at low frequencies due to reduced scattering and higher carrier mobility, while at higher temperatures, ϵ_2 decreases, reflecting increased scattering and reduced mobility. The frequency-dependent decrease in ϵ_2 aligns with the Drude model, which describes the optical properties of free carriers (electrons). In metals or semimetals, ϵ_2 is high at low frequencies due to strong energy absorption by free carriers, but it decreases as frequency increases and carriers are unable to respond to the rapid oscillations of the field efficiently.

Both ϵ_1 and ϵ_2 exhibit no temperature dependence at higher frequencies, where interband transitions or other intrinsic effects dominate over free carrier contributions. A clear transition from metallic to dielectric behavior is observed in ϵ_1 , while ϵ_2 diminishes, indicating reduced dissipation. This behavior is consistent with the Drude model, which successfully describes the low-frequency optical response in WP₂. Similar trends have been observed in other Weyl semimetals such as TaAs, NbAs, and WTe₂, where the low frequency dielectric response is dominated by free carriers, and interband transitions dominate at higher frequencies. Moreover, the trends in ϵ_1 and ϵ_2 are analogous to the corresponding real and imaginary parts of the conductivity (σ_1 and σ_2), as per the relationship:

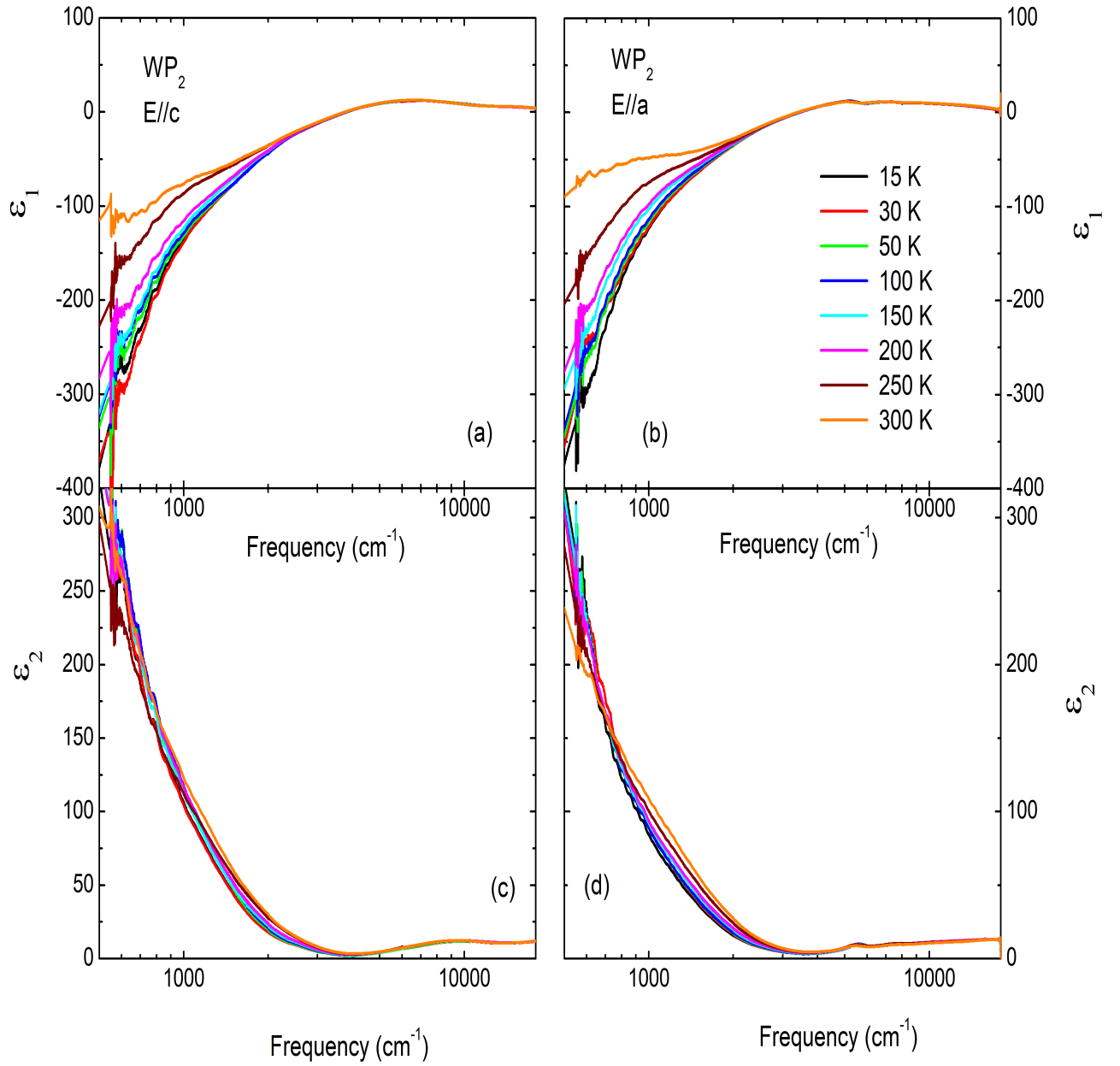


Figure 5.14: Frequency dependence of the (a) real part and (b) the imaginary part of the dielectric constant for $E//c$ axis plane with (c) the real part and (d) the imaginary part of the dielectric constant for $E//a$ axis plane.

$$\sigma(w) = i\omega\epsilon_0\epsilon(w) \quad (5.4)$$

The conductivity's real part aligns with the low frequency metallic screening in ε_1 , while its imaginary part mirrors the dissipation trends observed in ε_2 . In WP₂, the strong anisotropy between the a-axis and c-axis orientations is also a noteworthy feature, driven by the material's low crystal symmetry and the anisotropic distribution of Weyl nodes. This anisotropy results in direction dependent plasma frequencies and scattering rates, which are also consistent with optical investigations in other anisotropic Weyl semimetals.

Chapter 6

CONCLUSION

Tungsten diphosphide WP_2 , single crystal were investigated through resistivity and infrared optical spectroscopy reflectance measurements. The frequency dependent optical conductivity has been calculated from the reflectivity measurements and with the aid of Kramers-Kronig analysis. Using the calculated optical conductivity, spectral-weight analysis and extended Drude analysis have been performed. The results demonstrate that WP_2 exhibits exceptional properties, driven by its robust topological nature and anisotropic electronic structure, with significant implications for both fundamental physics and technological applications.

The resistivity measurements reveal a metallic behavior across the investigated temperature range with a saturation value at 2 K of $\rho \sim 2 \times 10^{-8} \Omega\text{cm}$ yielding high residual resistivity ratio (RRR) of up to 47,000, indicative of extremely high crystal purity and long electron mean free paths of WP_2 crystals studied here. At low temperatures ($T < 50$ K), the resistivity decreases sharply and shows a quadratic behavior pointing to Fermi liquid, due to reduced scattering mechanisms and the robust topological nature ensuring long carrier mean-free paths. This behavior aligns with hydrodynamic electron flow, a characteristic of WP_2 's unique electronic properties. At low temperatures (~ 10 K), resistivity becomes temperature-independent, suggesting residual resistivity dominance. This highlights WP_2 's high purity and unique topological properties that inhibit common scattering mechanisms. In contrast, at higher temperatures ($T > 200$ K), the resistivity displays a linear temperature dependence characteristic of electron-phonon scattering, highlighting WP_2 's metallic character.

The reflectivity spectra measured for $E // c$ and $E // a$ axis orientations, exhibit distinct temperature and frequency-dependent features. At low frequencies ($< 2000 \text{ cm}^{-1}$),

the reflectivity approaches unity for both orientation as temperature decreases, pointing to metallic behavior. The emergence of plasma edges at $\sim 3750 \text{ cm}^{-1}$ (E // c) and 3600 cm^{-1} (E // a) confirms the anisotropic plasma frequencies of WP_2 , a direct consequence of its low-symmetry orthorhombic structure. These edges are accompanied by valleys ($V_a \sim 3700 \text{ cm}^{-1}$ and $V_c \sim 4000 \text{ cm}^{-1}$), which highlight the anisotropy in the optical response. The valley ratio ($V_c/V_a \sim 1.2$) aligns closely with the theoretical predictions and supports the directional dependence of WP_2 's optical properties. Above 4000 cm^{-1} , an upturn in the reflectivity for both orientations is observed coupled with crossing points at specific frequencies. Such crossings are due to spectral weight redistribution.

The optical conductivity measurements of WP_2 , analyzed through Kramers-Kronig analysis, exhibit distinct behaviors along the crystalline axes, showing its anisotropic electronic properties. At low frequencies ($\omega < 1000 \text{ cm}^{-1}$), σ_1 shows a drude like response with minimal temperature dependence for both E // c-axis and E // a-axis orientations, reflecting robust charge carrier dynamics with limited scattering effects. Above 4000 cm^{-1} , the real part of the optical conductivity σ_1 , increases nearly linearly with frequency with a notable upturn for both orientations in the MIR ($4000 - 10,000 \text{ cm}^{-1}$) showing strong interband transitions. This linear behavior is attributed to WP_2 's linear band dispersion near the Weyl points and demonstrating spectral weight transfer between the two orientations.

The crossover frequencies where (σ_1) spectra for both orientations intersect ($\sim$ less than 1000 cm^{-1} and $\sim 10,000 \text{ cm}^{-1}$) for E // c - axis plane and ($\sim 1000 \text{ cm}^{-1}$ and $\sim 6000 \text{ cm}^{-1}$) E // a-axis, confirms spectral weight transfer from the MIR to low frequencies upon cooling. At the lowest frequency, the real part of the optical conductivity matches well with the DC conductivity values obtained from resistivity measurements pointing to the self consistencies of the optical data. The imaginary part of the optical conductivity (σ_2) decreases monotonically to zero above 3000 cm^{-1} for both orientations, which is consistent with reduced scattering and the high mobility of charge carriers, while higher frequency features associated with interband transitions, as evidenced by humps and valleys in the spectra are observed.

Spectral weight in WP_2 increases with frequency and becomes conserved beyond $\sim 10,800 \text{ cm}^{-1}$. At low frequencies ($< 1000 \text{ cm}^{-1}$), free carriers dominate, confirming WP_2 's metallicity with high carrier density ($\sim 2.5 \times 10^{21} \text{ cm}^{-3}$). In the mid-infrared ($1500 \text{ cm}^{-1} - 5000 \text{ cm}^{-1}$), spectral weight shifts from interband to intraband contributions at lower temperatures, enhancing carrier coherence. At high frequencies ($> 10,000 \text{ cm}^{-1}$), it saturates, following the optical sum rule. Extended Drude analysis shows a decreasing scattering rate at low frequen-

cies and temperatures, with a peak around 4000 cm^{-1} due to interband transitions. Effective mass values are low for both orientation i.e. $m^* = 0.8m_o$ for $E \parallel a$ -axis and $m^* = 1.2m_o$ for $E \parallel c$ -axis. This difference influences conductivity, as mobility ($\mu \propto \frac{1}{m}$) is higher along the a -axis. The lower effective mass along the a -axis suggests more dispersive bands, while the c -axis's slightly higher mass indicates less dispersive bands due to WP_2 's crystal symmetry. Despite differences, both values highlight the impact of topological properties near Weyl nodes, enhancing carrier mobility, reducing scattering, and contributing to high conductivity.

A unique feature of WP_2 is its anisotropic optical response. The anisotropy between the a -axis and c -axis orientations is reflected in both plasma frequencies and the spectral weight distribution, further corroborated by the distinct behaviors of σ_1 and σ_2 . Comparisons with other Weyl semimetals, such as MoTe_{22} and NbP , show similarities in band gap energies ($\sim 1.0 \text{ eV} - 2.0 \text{ eV}$) and spectral weight transfer, but WP_2 's unparalleled $\text{RRR} \sim 47\,000$ and hydrodynamic transport properties set it apart as a benchmark material.

The findings presented in this chapter elucidate the intricate interplay between WP_2 's topological properties, anisotropic band structure, and optical responses. The hydrodynamic transport regime at low temperatures and strong interband transitions at higher frequencies underlay WP_2 's unique position among type II Weyl semimetals. These results contribute significantly to understanding of anisotropic transport and optical properties in topological materials, paving the way for future explorations in electronic, spintronics, quantum computing, high-performance electronics, thermoelectrics, superconductivity, and optoelectronic applications.

Chapter 7

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