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Terahertz Time Domain Spectroscopy and Fresnel Coefficient Based Predictive Model

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TERAHERTZ TIME-DOMAIN SPECTROSCOPY AND FRESNEL COEFFICIENT BASED PREDICTIVE MODEL

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science

By

JUSTIN C. WHEATCROFT
B.S., Kent State University, 2009

2012
Wright State University
WRIGHT STATE UNIVERSITY

GRADUATE SCHOOL

August 31, 2012

I HEREBY RECOMMEND THAT THE THESIS PREPARED UNDER MY SUPERVISION BY Justin C. Wheatcroft ENTITLED Terahertz time domain spectroscopy and Fresnel coefficient based predictive model BE ACCEPTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF Master of Science.

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ABSTRACT

Wheatcroft, Justin C. M.S. Department of Physics, Wright State University, 2012. Terahertz time-domain spectroscopy and Fresnel coefficient based predictive model.

An optical material parameter predictive model that accounts for sample to air interfaces was developed. The model predicts how a terahertz time-domain spectroscopy time domain pulse will be affected as it passes through a given thickness of a material. The model assumes a homogenous, linear, isotropic dielectric or semiconductor. The inputs to the model are the real and imaginary refractive indices across the desired frequency band. Different dielectric material’s optical parameters were taken from the literature and the predicted time domain pulses were shown. It was also shown that the refractive index and absorption coefficient for samples that were optically thick and low-loss could be determined from measurements analytically. It was also shown that for non-dispersive media with a flat absorption coefficient, the predictive model could be used to determine an average value for both the index of refraction and the absorption coefficient across the frequency band, (0.1 – 4 terahertz).
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DEDICATIONS

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1. Introduction

1.1. General introduction to the contents of the thesis.

Terahertz (THz) radiation has been the focus of much study and research over the past 30 years [1-2]. Since 30 years is a relatively short time for a budding scientific concept or application, it allows for many groups or individuals to perform fundamental research and development. One such area of research is the electrical (or optical) characterization of materials at THz frequencies. Unlike other well known frequency bands (such as infrared, microwave, optical, etc.) where material characterization has been going on for many more years than for THz frequency light, there are many fundamental research opportunities that are available to researchers. For example, researchers who utilize other frequency bands are generally restricted to unconventional media and complicated designer materials because a large majority of simple dielectrics and semiconductors have been thoroughly characterized [3]. This is not the case for most materials in the THz regime, where fairly standard and homogenous materials still need to be properly (and repeatedly) characterized at THz frequencies.

This begs the question, “if materials have been thoroughly characterized in other well-known frequency spectrums, then why go to all the bother characterizing in the THz band?” Simply put, many organic, semiconductor, and dielectric materials exhibit interesting resonance properties at THz frequencies. Also, knowing the electronic properties of these materials is important due to the development of electronic devices
that operate at these frequencies. This makes THz radiation ideal for characterizing such materials. THz radiation is also non-ionizing, which makes it extremely useful for non-destructive and non-evasive imaging. To accommodate (and capitalize on) this growing field of research, companies such as Teraview (www.teraview.com) and Picometrix (www.picometrix.com) have tabletop continuous wave (CW) and time domain (TD) THz systems available for purchase. In the case of the Teraview THz TD system, it can effectively generate a clean frequency spectrum from 0.1-5 THz at the push of a button. These types of systems have greatly increased the knowledge and functionality of the 0.1-5 THz portion of the electromagnetic (EM) spectrum.

There are some fundamental reasons why THz research did not occur at roughly the same time as research into other frequency bands. First and foremost, THz radiation is readily absorbed by atmospheric water vapor. Figure 1-1 below shows the absorbance spectrum of water vapor from 0.5 – 2.5 THz [4]. The first three peaks (at 0.558, 0.753, and 0.996 THz respectively) are highlighted for clarity. This water vapor absorption prohibits the use of THz radiation as a broadcast telecommunications source. That is why broadcast and radar systems have frequency ranges from VHU/UHF up to roughly 30 GHz, because radiation at these frequencies does not get absorbed by water vapor. However, there are free-space THz systems that are designed to account for this issue, such as THz Doppler radars [5], and emerging THz short-range communication devices [6]. Also, when performing table-top material characterizations at THz frequencies, the area where the THz radiation propagates can be encapsulated and all the air, and therefore the water vapor, can be evacuated (leaving a vacuum), or a gas such as N₂ can be pumped in, which does not absorb THz radiation.
Figure 1-1: Absorbance spectrum of water vapor (with the first three peaks enlarged) [4].

Another issue with THz systems is that high power THz radiation is difficult to produce. Many of the THz generation techniques (described below) are relatively low powered because the antennas and non-linear optical (NLO) crystals used for THz generation will undergo dielectric break down at higher input powers. The purpose of having a high power output is to broaden the gap between the measured signal and the noise floor. Of course, both signal and noise will increase with power; however they both do not increase at the same rate. This means that the gap between them will increase up to a point. Depending on many factors (like devices used and cabling/connections as some examples) there will be a point where other techniques must be used to lower the noise floor.

Even with the limitations described above, there are many good reasons to investigate the THz region. First and foremost is material characterization. To understand
how a material behaves optically, one must know the material’s complex index of refraction (at the desired frequencies). The complex index of refraction ($\tilde{n}$) is an intrinsic property specific to any given material that is utilized when taking an optical approach for determining how an electromagnetic wave interacts with that material. The complex index of refraction is the main material parameter of concern for this thesis. Of course, optics is simply an electromagnetic theory, and $\tilde{n}$ is defined in terms of the electrical material parameters: complex permittivity ($\tilde{\varepsilon}$) and permeability ($\tilde{\mu}$). Simply put, to understand how a material behaves optically or electrically at THz frequencies, one must know either $\tilde{n}$, or both $\tilde{\varepsilon}$ and $\tilde{\mu}$. This information could lead to a material’s conductivity, and even the electron mobility in the case of a semiconductor.

Some material’s structures will interact with a specific frequency, sometimes exhibiting higher energy absorption at and around that specific frequency. These materials possess what is known as a phonon resonance. Phonons are the periodic vibrational modes of the constituent particles within a structured material (such as a crystal) that only occur when energy of a specific frequency propagates through the material. A phonon is not a particle itself, but is a quasi-particle, which means that phonons exhibit certain properties and can be treated as if they were a real particle. Phonon resonances in materials at THz frequencies often correlate to an absorption peak seen in the spectrum. Not all materials have phonon resonances at THz frequencies; however some dielectrics, semiconductors, and man-made structured materials do. For example, dielectrics such as zinc telluride (ZnTe) and cadmium telluride (CdTe) have phonon resonances at 5.31 and 4.31 THz respectively [7]. The crystal structures of these materials vibrate at a specific frequency, which in-turn absorbs the part of the energy at
that frequency. These spikes in the frequency spectrum (or absorption coefficient) can be thought of as a “fingerprint” since they are fairly unique to each material, and aid in the characterization of these materials. Work has been done that shows that THz spectroscopy can differentiate between types of illicit drugs [8]. This research focuses on non-destructive imaging through luggage and of persons at THz frequencies, looking for the spectral fingerprints of illegal substances.

The THz regime is lacking in semiconductor devices that perform similar roles to those that are utilized in the radar and infrared (IR) frequency bands. As discussed above, this lack of THz related devices is due simply to the fact that comparatively, THz research is fairly new. As an example, the development of broadband (0.2 – 15 THz) bandpass filters occurred fairly recently [9-10]. Generally speaking, these bandpass filters are structured materials that have a resonance at the desired frequency, but these first generation devices operated over a very limited bandwidth (0.2 – 3 THz). Only through recent developments in frequency selective surfaces (FSS), i.e., metamaterials (MM) has the usable bandwidth of these devices increased to what it is today [11].

There are two important aspects associated with classifying a material’s electrical and optical properties: measurement and modeling. A well known and controlled system is critical to the measurement process. This will provide not only a system with limited measurement error, but a means in which to mathematically equate measurements to known variables. Also, realistic models of the interactions between the sample and the electric field are equally as important as a functioning measurement system. The models provide a means to relate the measurements to bulk electrical properties of the samples under test. The second portion, and the majority of this thesis involves developing an
accurate model for predicting how a terahertz pulse will be affected by a known material as it propagates through it. This predictive method can then be used to determine an unknown material’s optical parameters either manually or by using an iterative solver. The modeling process is discussed in chapter 3 and the results are discussed in chapters 4 and 5.

1.2. Measurement System and Modeling Introduction

Measuring the frequency-dependent material properties such as the index of refraction and optical absorption play a key role in identifying materials as described above. One such novel method is terahertz time domain spectroscopy (THz TDS) [12-13]. This method uses an extremely short terahertz time domain pulse to generate a broad frequency spectrum. The terahertz pulse is on the order of sub-picoseconds in width (in reference to the speed of light). A reference measurement is taken in which the THz pulse travels through a free-space path either in air or vacuum (see Figure 1-2).
A sample is then put in the path of the THz pulse and a measurement is taken. The two different measurements can then be used to extract the various material parameters (discussed above) from the measured sample. Generally this comparison is done in the frequency domain, since the mathematics simplifies to division and multiplication (Eqn. 1.1) instead of the more grueling convolution integrals needed for time domain analysis (Eqn. 1.2).

\[
y(\omega) = x(\omega) \times h(\omega) \tag{1.1}
\]

\[
y(t) = \int_{-\infty}^{\infty} x(\tau) h(t - \tau) d\tau \tag{1.2}
\]

The frequency spectrum produced has both amplitude and phase information. The two measured quantities can then be used to determine two independent material parameters over the entire bandwidth of the measurement. As discussed above, the real and imaginary part of the index of refraction can be determined. For this thesis, the
imaginary part of the index of refraction is put in terms of absorption. The two quantities are related by a simple algebraic expression (where \( c \) is the speed of light in a vacuum and \( \omega \) is the angular frequency.

\[
n_t(\omega) = \frac{\alpha(\omega)c}{2\omega}
\]

This change is done because the community is more concerned with how a material attenuates a propagating EM wave based on loss at specific frequencies. Absorption relays that information directly. As stated above, any two independent material properties can be determined, not just the complex index of refraction. Other possible material parameters include the permittivity, permeability, and even sample specific properties such as sample thickness [14-16].

Extracting a material’s constituent properties from a measurement requires a valid model. For a model to be considered valid, it must sufficiently relate the desired material parameters to the measured data in such a way as to not violate accepted scientific principles. A model must also correctly and accurately describe the specific interactions that are occurring. For instance, when electrical radiation encounters an interface between two adjoining materials, some of the radiation transmits through, while some radiation reflects backwards. The most simplistic models do not account for reflection losses, but are designed only to account for radiation passing through the material under test. Slightly more accurate models account for the radiation losses at each interface due to reflections. More complicated and accurate models account for multiple reflections within the sample that eventually transmit through. The main goal of this thesis was to develop a model that accounted for all the losses and reflections.
1.3. Description of THz, definitions and uses.

The Terahertz (THz) frequency band lies between the mid-infrared and millimeter wave portion of the electromagnetic (EM) spectrum, roughly 0.1-10 THz. It resides between the portions of the EM spectrum that are generally described using their wave-like characteristics (microwave regime), and their particle-like characteristics (infrared). This frequency bandwidth corresponds to wavelengths ranging from 0.03-3 mm. Due to its position on the frequency band, THz radiation is sometimes referred to as sub-millimeter or far-infrared. It is also widely known as the “Terahertz gap”, which is a reference to the lack of efficient and effective technology in this frequency range. It has proven difficult to produce effective (and inexpensive) emitters, detectors, and systems in this range [17]. A simplified EM spectrum (given in hertz) is shown in Figure 1-3 below [18].

![Figure 1-3: Electromagnetic Frequency Band](http://www.rpl.edu/~zhengjc/)

Figure 1-3: Electromagnetic Frequency Band [18]
THz radiation has some interesting characteristics. Using Planck’s relationship between energy and frequency, photons at THz frequencies are relatively low energy compared to higher frequency radiation.

\[ E = hf \]

The energy of a photon at THz frequencies is insufficient to ionize atoms. Ionization of an atom is when a photon carries enough energy to completely remove an electron from an atom or molecule. Since THz radiation is non-ionizing, it is particularly useful when dealing with organic materials. Unlike X-rays, which carry enough energy in its photons to ionize organic tissue, THz radiation does not. To this end, research is being done to utilize THz radiation as an alternate organic tissue imaging technique [19]. Of course, the absorption of THz radiation due to water (abundant in organic tissue) is a major issue that needs to be addressed before this becomes a practical alternative to X-ray radiation.

A large majority of non-conductive (dielectric) materials are either completely or moderately transparent to THz radiation. This list includes (but is not limited too), some plastic, cloth, some ceramics, paper, and some organic matter. On the other hand, metals reflect THz very well. Figure 3 is a THz image of the contents of a closed polyester briefcase. This image was taken by Wright State University students Satya Ganti and Michael Molton using the Teraview time domain system and the imaging gantry. The Teraview can be used in an external mode, where two fiber optic modules can generate and detect their own THz signal. The image gantry is a 3-D raster scan setup; however this image was taken in only two dimensions. The time domain wave form was measured
at each pixel as the modules were moved from position to position. The image was based on the amplitude of the time domain pulse at each pixel. The briefcase is transparent to the THz radiation, so the contents that are within become readily visible. Also seen in the picture are the contents of a plastic CD case that is also within the briefcase. The image was taken in transmission mode, which is why the metallic objects appear black, since they did not allow any radiation to pass through them to the detector.

![Image of a terahertz image taken of the contents of a close leather briefcase.](image)

**Figure 1-4:** A terahertz image taken of the contents of a close leather briefcase.

THz-TDS imaging has been explored since the early 1990’s, but difficulties in generating and detecting THz prevented any real breakthroughs until the 1995. One of the first recorded THz images was taken at AT&T Bell Labs by B.B. Hu and M.C. Huss in 1995 [20]. This was done using a terahertz time-domain spectroscopy (THz-TDS) setup that performed a raster scan of the object. The transmitted waves were down-converted into a kilohertz (audio) signal and processed using a digital signal processor.
This device would display the spectral data of the scan, which in turn generated the images seen in Figure 1-5.

![Figure 1-5](image)

**Figure 1-5: Some of the first images ever recorded using THz radiation. Top shows a semiconductor integrated circuit imaged through plastic packaging, and bottom shows two images taken of the same leaf 48 hours apart. Water content within the leaf can be determined [20].**

THz radiation is also extremely useful for characterizing materials. As described above, many materials are being characterized at THz frequencies. Also, many solids, liquids, and gases exhibit specific absorbance peaks within the frequency band. These peaks act as a sort of “THz fingerprint” for identifying the substance under test. For instance, water vapor has a very specific absorbance spectrum, which can be detrimental to the utility of a free-space THz device (see Figure 1-1 above). Semiconductors and polymers exhibit interesting frequency dependent conductivities and permittivities.
Having these conductivity and/or permittivity profiles proves especially useful in characterizing these materials at THz frequencies.

1.4. Roadmap for the document

The overall purpose of this thesis is to provide a more realistic model for THz TDS systems. This model takes into account interface losses and multiple internal reflections for dielectric and semiconductor materials with and without loss. Chapter two provides a background concerning THz TDS and its uses. Chapter three is the longest chapter, and it deals with the development of the EM model. It begins with a background into E&M, defines the different electrical material parameters, and discusses how waves propagate through a material (using ray optics). Then, starting with the simplest case, a formula is developed relating the transmitted electric fields to the material parameters. Lastly, the derived formula for the simple case is inverted to determine material parameters based on measured fields. Chapter four discusses in detail the simplest case (optically thick samples with little to no loss) and compares the model to measured data. Also, the simple model is extended to account for reflection losses at the air/sample interfaces, but this is only done for the low loss case. A simple uncertainty analysis centered on thickness variation is also performed as well. Chapter five discusses the more complex case of optically thin and lossy systems. The model is used and compared to a known sample. It is shown how the model can be used to determine what the index of refraction and absorption of a sample is across the frequency band. Chapter six is the conclusion, discussing the validity of the developed models and outlines what future work needs to done. Lastly, chapter seven is the list of references, and the MATLAB code written in conjunction with this thesis is provided in the appendix.
2. Background

2.1. Introduction

Terahertz time domain spectroscopy (THz TDS) is a measurement technique that is used for determining intrinsic electronic and optical properties of materials in the THz frequency range. As its name states, THz TDS is a spectroscopic technique that uses ultra-short pulses of terahertz radiation to probe materials. The pulse width is generally on the order of less than a picosecond, which can then be transformed into a broadband spectrum in the frequency domain using a discreet Fourier transform, (specifically the Fast Fourier transform). A THz pulse (Figure 2-1 and Figure 2-2) and frequency spectrum (Figure 2-3) are shown below.

Figure 2-1: Time domain THz pulse.
Figure 2-2: Zoomed in view, highlighting the multiple pulses seen from the sample measurement.

Figure 2-3: THz frequency domain plot.

Essentially, the frequency-dependent amplitude and phase of a reference signal (no sample in place), and a sample signal can be used to extract the unknown electronic
and optical properties of the material under test. This chapter will discuss the basics of THz TDS, explaining typical system components and measurement procedures.

2.2. Need for THz spectroscopy.

As discussed above, THz TDS systems utilize an ultra-short terahertz pulse to probe materials and aid in the extraction of bulk electronic properties of said materials. By Fourier optics (or Heisenberg’s Uncertainty Principle), the shorter in time the THz pulse is, the broader the frequency response will be. This is of course limited by many factors, including generation and detection methods and optical dispersion. Typical THz TDS spectra can range from 0.1 – 4 THz.

As discussed in Chapter 1, it is important to understand how materials electronically or optically behave at THz frequencies for many reasons. From a material science standpoint, determining materials for use in THz applications requires knowing the material’s electronic and optic parameters. This includes the complex index of refraction (real part and the absorption). Knowing these can lead to the material’s complex permittivity and permeability, as well as conductivity (for semiconductors as an example) [14-16]. Characterizing materials is tantamount to the research and development of THz electronic devices. Also, many materials have unique phonon resonances in the THz regime, which proves useful in many THz applications, such as material identification and the creation of THz devices (both discussed in chapter 1) [7]. To this end, THz TDS is a useful tool for determining these material properties. Its utility is in the fact that it is a broadband measurement. The constituent material parameters can
be measured over the entire bandwidth of the device instead of at a single frequency point as with continuous wave (CW), or frequency domain systems. For materials with phonon resonances at THz frequencies, THz TDS systems can determine not only the associated frequency, but how much the incident signal is attenuated, and how wide (in frequency) the attenuation is [21-22]. There are other devices, such as Fourier transform interferometers (FTIR), which have large spectral ranges, but they are only able to provide amplitude information. To obtain the phase information one must use complicated Kramers-König relations, which makes FTIR devices undesirable.

Many materials (such as polymers, plastics, etc.) are transparent to THz radiation. This has obvious implications for THz imaging through these materials, such as imaging inside a visibly opaque plastic case to determine its contents. THz TDS can be used to determine the material properties of these materials. One such use for this information is for developing THz related components, such as liquid or gas sample holders and inexpensive plastic lenses.

Another benefit to using THz TDS is that THz radiation is non-ionizing. This means that biological samples can be measured at THz frequencies without adversely affecting the sample. For example, THz TDS of bone samples is providing researchers with ex-situ information on bone density [23]. The absorption spectrum of the bone is analyzed, using that information to determine if there is a relationship between the density of the bone and the amount of water in the bone. Cancer research has been performed using THz radiation sources, taking advantage of the fact that non-ionizing radiation will not affect the samples, but also of THz radiation’s water absorption spectra [24]. Some preliminary research has shown that skin cancer cells, having different water
content than healthy skin, can be detected much earlier in the onset than with traditional detection methods [24].

2.3. Typical THz TDS setup and components

The THz TDS system used for this effort was the Teraview Spectra 3000. It has the capability to measure samples in free-space, or in an air purged environment. It can accommodate both transmission and reflection measurements, and also has on-board software that will operate the system, as well provide material parameter extractions for measured materials. Described below are the various components used in the Teraview system used for this effort. In general, many of the components used on the Teraview are similar to many components used in other THz TDS setups. There are exceptions, and some of these exceptions will be discussed in the following section. The major components used in the Teraview will be described in more detail, with only a short description and references for further research provided for alternate components.

A typical THz TDS setup is shown below in Figure 2-4 [25]. The first component shown in the diagram is the ultrafast pulsed laser. Ultrafast optics is a field of study that centers on the generation, detection, and utilization of femtosecond pulsed laser light [26]. There are a few different methods for generating an ultrafast laser pulse, but the most popular method, and the method used in the Teraview system is through Kerr lens modelocking [27]. This method utilizes a continuous wave laser (532 nm for a doubled Nd laser) and a titanium doped sapphire crystal (Ti:saph) [27]. The optical cavity of the laser acts as a resonator, with an output coupler that allows some energy to
pass out of the system [27]. The continuous wave laser pumps the Ti:sapphire, producing laser light with a 800 nm wavelength. This 800 nm light passes back and forth through the cavity, passing through the titanium sapphire crystal at each pass. The titanium sapphire crystal acts as a gain medium for the 800 nm laser light. The crystal produces a Kerr effect in the laser light. The crystal’s index of refraction changes as a function of laser light intensity. As the light (which is shaped as a Gaussian) passes through the crystal, the variation in intensity causes the index of refraction to vary throughout the crystal. This in turn focuses the light, a nonlinear process known as Kerr lensing [28].

The intense laser light traveling back and forth through the laser cavity is comprised of multiple modes. Even though the laser pumping the titanium sapphire crystal is continuous wave, it is still comprised of a certain number of frequencies. Some of these modes will produce standing waves inside the laser cavity (generally those with wavelengths or half wavelengths that are an integer number of the total length of the cavity) [27]. Other waves will destructively interfere with themselves and other non-standing waves, and nearly cancel themselves out. These different modes of standing waves will interfere with one another, and produce a very short pulse of laser light [27]. The ultrashort pulse width and the frequency in which they are produced depends on the center wavelength of the continuous laser, the optical components used, and the laser cavity geometry.
The ultrafast pulsed laser fulfills two needs of the system. First, it is used to generate the THz pulse in either a photoconductive (PC) antenna or through an electro-optic (EO) crystal. The Teraview system uses a PC antenna, so EO generation techniques will not be discussed here but the technique is thoroughly described in Dr. Ruffin’s doctoral thesis [29]. A PC antenna consists of two biased metal electrodes (dimensions shown) and a semiconductor substrate, as seen in Figure 2-5 [30]. A typical substrate used for detection antennas is low temperature grown gallium arsenide, or LT GaAs [9]. This material is used primarily because the low temperature growth results in a very fast carrier trapping time, which provides the detector with a small time resolution [30].
Figure 2-5: Diagram of a stripline and dipole photoconductive antenna (top). Optimal location for ultrashort laser pulse (bottom) [30].

The ultrashort laser pulse strikes the semiconductive substrate between the striplines or dipole antennas. As long as the energy of the incident laser pulse is greater than the band-gap energy (1.43 eV at 300K for GaAs), free electron and electron hole pairs are produced in the semiconductor substrate. The biased electrodes accelerate the free carriers for the time the pulse is hitting the antenna, which is the same time as the width of the pulse. This acceleration of the electrons produces the sub-picosecond electromagnetic fields, which are the THz pulses [30].

Going back to Figure 2-4 above, before any THz pulses are produced, the ultrashort laser pulse is split into two separate beams. The pump beam is responsible for the generation of the THz pulse as described in the previous paragraph. The second beam is referred to as the probe beam. This part of the ultrashort pulse is responsible for measuring the generated THz pulse. As with THz pulse generation, there are multiple THz detection techniques. The Teraview system used a PC antenna for detection as well; however EO detection methods exist, and one such method is also described in the doctoral thesis mentioned in the previous paragraph [29]. Also described in the same
thesis is the PC antenna detection technique. Both the emitting and detecting PC antennas have a collimating or hyper-hemispherical lens attached to them. For the emitting antenna, the dome lens helps couple out the THz radiation from the semiconductive substrate into free-space; collimating the beam as it passes through the lens. For detection schemes, this lens admits the collimated THz light, focusing it down onto the antenna gap [31]. Now, referring to Figure 2-6, the PC antenna detects the THz pulse much like it generates it, only in reverse. Instead of biasing the metal electrodes, they are instead attached to an ammeter. The incident THz pulse produces a current in the gap between the electrodes only when the semiconductive substrate is excited by the ultrashort optical pulse [32]. The lifetime of the free carriers is directly related to the ultrashort pulse width; which in turn is much shorter than the duration of the THz pulse. This will in turn sample the THz pulse as the time in which the ultrashort pulse hits the PC antenna is varied (discussed below). Also, since the electrical bias in the metal electrodes is due to the incident THz pulse, then the induced current is proportional to the amplitude of the portion of the THz pulse that is currently being sampled.

![Figure 2-6: Photoconductive antenna THz detection scheme.](image)

As stated above, the time in which the ultrashort pulse is incident on the PC antenna is varied by means of an optical delay rail. The delay rail is simply a set of
mirrors that are set along the path of the probe beam, but are connected to a motorized stage. The stage is then moved a set distance, and a measurement is taken. This process is repeated until the entire THz pulse has been sampled. The optical resolution of the system is then defined by the width of the ultrashort pulse, which is on the order a hundred femtoseconds. Figure 2-7 is a schematic of the ultrashort pulse scanning the THz pulse. The ultrashort pulse can be thought of as a sinc function. This analogy works well, because the THz pulse should be sampled in independent pieces, where the ultrashort pulse does not overlap between measurements. Therefore, for optimum sampling and the finest resolution, the delay rail should be moved in micron steps.

![Figure 2-7: THz pulse being sampled by the ultrashort laser pulse.](image)

Sample placement in a THz TDS system occurs within the THz pulse beam path. There are many different setups, and they depend on what types of samples are being measured. If sample size is an issue, then focusing and collimating mirrors called parabolics, or lenses made out of high density polyethylene (for example) are used to focus the THz pulse onto the sample, and then re-collimate the beam to be measured at
the detector. If there is no need or desire to focus the THz pulse, then a direct illumination and detection method can be used. In this case, the sample is placed directly between the transmit and receive antennas (or EO crystals). Gas purging chambers can also be used for either setup. A purging chamber is used to evacuate the air (which contains water vapor) by filling the sealed chamber with nitrogen ($N_2$). The $N_2$ gas does not readily absorb THz radiation like water vapor does, so a cleaner frequency spectrum (without the water lines discussed in chapter 1) can be obtained. Another consideration is whether transmission or reflection measurements are desired. In either case, there is a separate device for transmitting and receiving the THz pulse, which means that boresight reflection measurements cannot be done unless a beam splitter is placed in the path of the THz pulse. This configuration was not utilized with the system described in the thesis.

2.4. Description of Teraview system specifics

The measurements performed for this thesis were done on the Teraview TPS Spectra 3000. This system has both an internal measurement chamber, and an external fiber-optic module measurement setup. The internal measurement chamber is set up similar to the diagram above and can only measure in transmission mode. The sample chamber can be purged of air by filling it with $N_2$ as described above. This can greatly reduce the “clutter” from atmospheric water.

The fiber optic modules transfer the ultrafast laser pulses to the external set of PC antennas. These external modules can be used for reflection and transmission measurements of samples, THz imaging (in reflection or transmission), and scattering measurements. Teraview’s website quotes a spectral range of 0.06 – 3 THz, although the
system has successfully reached 4 THz. Their website also boasts that it is the world’s first commercially available THz spectroscopy system [33]. A three axis imaging gantry can also be purchased, and this same gantry was used to take the briefcase image shown in Figure 1-4. The Teraview comes with a Windows based operating system, and a software suite that is used to operate the system, performs measurements, and even does simple material parameter extractions. The extractions performed are only for lossless and optically thick samples. Other more complicated samples can be measured and the extraction software can be used; however the extracted values will not be accurate. A more thorough discussion into the extraction process and the inherit errors is withheld for chapter 3. All measurements performed and presented below were not done under purged conditions, but were done within an open sample chamber.

2.5. Conclusion

THz TDS is a measurement technique that can be utilized for broadband characterization of materials, as well as imaging at THz frequencies. There are many different THz generation and detection techniques, but the Teraview Spectra 3000 THz TDS system uses PC antennas for both detection and generation. The system can be used in its chamber mode, which can be purged of all water vapor, or the system can be used in external mode, allowing for more measurement setup variation and larger sized images.

This thesis is concerned with the characterization of materials using a THz TDS setup. Understanding how this system functions, and how the energy propagates through
the system is tantamount to being to use the information gathered for material characterization purposes. To this end, chapter three describes the electromagnetic properties of the THz pulse produced by this system. It uses this information to describe how these pulses interact with isotropic, homogenous slabs of material.
3. Electromagnetic Background and Model Development

3.1. Introduction

Any good measurement device is rendered useless without an accurate model relating what is physically occurring during measurement to the desired material parameters. The THz TDS system generates a plane wave that interacts with the sample, which is simple enough in itself to model [34]. Problems arise when considering the interactions between the incident wave and the material. Many things need to be considered. First, what is known about the material? Second, how is the wave incident on the material, i.e. what is the wave’s polarization, what is the angle of incidence, etc. Lastly, what possible error sources are involved? This chapter describes in detail the electromagnetic theory involved in generating an accurate and realistic model of the planar THz wave as it propagates through a rectangular slab of material. The methods and intermittent equations used in the derivation process presented below were heavily borrowed from the Hecht *Optics* textbook [35]. This includes looking into how electric fields interact with matter, and what electronic and optical parameters are of interest. Also, a discussion on ray optics and Fresnel losses will lead into the development of the model.
3.2. Electric fields in matter.

As stated previously, the electromagnetic wave can be approximated as a plane wave [34]. For a plane wave, the electric field can be written as:

$$\vec{E} = \vec{E}_0 e^{i(k \cdot r - \omega t)}$$  \hspace{1cm} (3.1)

where $\vec{k}$ is the propagation vector, $r$ is the position of the wave in 3-dimensional space, $\omega$ is the angular frequency, and $t$ is the time. The THz pulse is only traveling in one direction as it passes through the sample. Therefore, the dot product in equation 3.1 can be reduced to a product of two constants.

$$\vec{E} = \vec{E}_0 e^{i(kx - \omega t)}$$  \hspace{1cm} (3.2)

The above field is considered propagating through free-space, or in other words a vacuum. However, when waves interact with an isotropic homogenous material multiple things occur. First, the wave’s phase velocity is reduced. The electric field interacts with the material on a microscopic scale, being absorbed and retransmitted as it passes through the material. Electric and magnetic fields through matter can be shown via the following expressions.

$$\vec{D} = \varepsilon \vec{E}$$  \hspace{1cm} (3.3)

$$\vec{H} = \mu \vec{B}$$  \hspace{1cm} (3.4)

$$\vec{j} = \sigma \vec{E}$$  \hspace{1cm} (3.5)
The “constants” $\varepsilon$, $\mu$, and $\sigma$ are the permittivity, permeability, and conductivity of a material (respectively). These values vary with frequency; however, for free-space the values are constant at all frequencies. Also, the above representation of the electromagnetic parameters is in an absolute form, but generally the permittivity and permeability are presented in a relative form (relative to free space).

\begin{align*}
\tilde{\varepsilon} &= \varepsilon' - j \varepsilon'' = \varepsilon_0 \tilde{\varepsilon}_r \quad &\text{(3.6)} \\
\tilde{\mu} &= \mu' - j \mu'' = \mu_0 \tilde{\mu}_r \quad &\text{(3.7)}
\end{align*}

The two constants in equations 3.6 and 3.7 have been measured to be $\varepsilon_0 = 8.854E-12$ farads per meter, and $\mu_0 = 4\pi E-7$ henrys per meter (in SI units), and are the permittivity and permeability of free space respectively. There is no such relation for conductivity, because the conductivity of free space is zero. All three electromagnetic parameters are also complex, having real and imaginary components (with free space having only real parts). However, the conductivity as it is defined and utilized here is strictly a real number. For $\varepsilon$, and $\mu$ the real parts relate to how well aligned electric and magnetic dipoles align in a material as an electric field passes through it. The imaginary components represent energy loss (generally in the form of heat), from the work done aligning the electric and magnetic dipoles. The conductivity represents how well an electric current will travel through a material. In a conductor, there are a number of free electrons that allow the current to flow through the material; whereas in a dielectric there are no free electrons (thus a conductivity of zero).

Generally, in optics, the index of refraction is used to describe how light passes through a material. There is a simple relationship between the above electric material
parameters and the index of refraction. Starting with the definition of an electric field’s phase velocity through a material based on the permittivity and permeability:

\[ v_p = \frac{1}{\sqrt{\varepsilon \mu}} \]  

and the definition of the index of the refraction, as the phase velocity of a light wave in relation to that in a vacuum, the relationship between index of refraction and permittivity and permeability is presented below.

\[ n \equiv \frac{c}{v_p} = \sqrt{\frac{\varepsilon \mu}{\varepsilon_0 \mu_0}} \]

The complex refractive index is similar to the complex permittivity and permeability, in that the real part accounts for how fast light can travel through a material; while the imaginary part pertains to the amount of loss, or absorption, in the material. Essentially, the complex index of refraction is to light as the complex permittivity is to an electric field. Determining the complex index of refraction would simply entail including the real and imaginary components of the permittivity and the permeability in the above relationship. For instance, in a non-magnetic material (complex \(\mu_r\) is equal to 1), the index of refraction is related to permittivity as follows.

\[ \bar{n} = n_R - i n_I = \sqrt{\varepsilon_R - i \varepsilon_I} \]

It is useful to note that the material parameters defined above are essentially only for bulk (macroscopic) materials. The formalism used to define them only incorporated the fields and currents through matter as a bulk substance. However, in some cases it is
more useful to talk about the way light and energy interact with matter on the microscopic scale. One such quantity is known as dispersion. Dispersion is the phenomenon in which the refractive index of a material is dependent on frequency. This was touched on above, but to truly understand the importance of dispersion, one must apply it to the microscopic structures of the material. Every material (besides vacuum) is dispersive. The dispersion is directly related to the square of the index of refraction, (based on the Drude model), and assumes a homogeneous material.

\[ n^2(\omega) = 1 + \frac{Nq_e^2}{\epsilon_0 m_e} \left( \frac{1}{\omega_0^2 - \omega^2} \right) \]  

3.11.

In the equation above, \( N \) is the electron density, \( q_e \) is the charge of an electron, \( m_e \) is the mass of an electron, and \( \omega_0 \) is the resonant frequency of the electrons within the material. It is obvious from this equation that the index of refraction changes as a function of frequency. An example of the importance of the above equation is the design of optical components for ultrafast laser pulses [36]. The ultrashort pulse width must be maintained throughout the entire optical pathway. Unfortunately, dispersion due to the optical components will skew (referred to as chirping) and broaden the pulse as it interacts with it. Ultrashort pulses in time have very broadband responses in the frequency domain, which means (looking at 3.11 above), the different frequencies will all have different indices of refraction. This means that the different frequencies will be traveling through the material at different rates. This can be compensated for by the use of negative dispersive materials that will chirp the pulse in the opposite direction. A more detailed discussion on the effects of dispersion and how to compensate for them was presented by X. Gu et.al [37].
It is also useful to define the conductivity of a material in terms of the permittivity. This is a novel method for determining the conductance of a semiconductor. Going back to the time-harmonic Maxwell equations, the curl of the magnetic field can be shown in terms of the equations 3.3 and 3.5 (assuming non-magnetic).

\[ \nabla \times \mathbf{H} = \sigma \mathbf{E} + j \omega \varepsilon \mathbf{E} \quad 3.12. \]

Using the definition of permittivity from equation 3.6 and plugging the real and imaginary part into the previous equation yields:

\[ \nabla \times \mathbf{H} = \sigma \mathbf{E} + j \omega \varepsilon' \mathbf{E} - \omega \varepsilon'' \mathbf{E} \quad 3.13. \]

The real part of equation 3.13 has both the conductivity and the imaginary part of the permittivity. This effective conductivity is the combined conduction and dielectric losses from a material; which shows that the two cannot be distinguished.

\[ \sigma_{\text{eff}} = \sigma - \omega \varepsilon'' \quad 3.14. \]

Now that the correlations between the various material parameters have been defined, it is feasible to measure some and obtain the others. This thesis is concerned with the complex index of refraction, and the rest of this chapter will be developing a relationship between those parameters and the measured electric fields. However, one can now easily find other electric material parameters by using the relationships derived above.
Going back to equation 3.9 and the definition of \( k \) in terms of phase velocity, a relationship for the electric field passing through a material in terms of index of refraction can be determined. The wave number \( k \) is given by:

\[
k = \frac{\omega}{v_p}
\]

which when inserted into equation 3.2 gives the following equation (propagating in the positive \( x \) direction).

\[
\vec{E} = \vec{E_0}e^{i\omega(xR/c - t)}
\]

Inputting the full complex form of the index of refraction will give the following relationship.

\[
\vec{E} = \vec{E_0}e^{-i\omega \frac{n_1}{c}}e^{i\omega(t - \frac{xR}{c})}
\]

Now that the field equation that defines the electric field of a light wave propagating through matter has been developed in terms of the complex refractive index, a simple model can be developed that utilizes this relationship. The simple model is simply the THz pulse passing through a low loss optically thick material. A low loss material has an imaginary index of refraction that is much smaller than the real part. Speaking in relative terms (\( \tilde{n} \)), a material is considered low loss when the imaginary part is at least an order of magnitude smaller than the real part. An optically thick sample is one such that the Fabry-perot reflections do not contribute to the overall signal. When light is incident on an interface between two different mediums, some of the light is reflected and some is transmitted. Some of the reflected light will be reflected back in
the direction of propagation (towards the detector). In one case, the thickness and refractive index of the material only allow a single THz pulse to reach the detector within the measurement time window. As an example, suppose the time window of the THz TDS system is 100 ps in length, and the sample being measured has a real index of refraction twice that of air. If the sample was larger than 500µm in length, no multiple reflections would reach the detector in time. The second pulse to reach the detector would have to travel through the material three times, which would put it just at the end of the time window (see equation 3.18).

\[
\text{time}_{\text{pulse 2}} = \frac{\text{total length traveled}}{\text{speed of light through material}}
\]

\[
\text{time} = \frac{3 \times \text{thickness}}{c_0/n} = \frac{3 \times (5E - 3)}{(2.99E8)/2} = 100.3 \text{ ps}
\]

The second case is when there are multi-pass signals that reach the detector within the measurement window, but the signals are attenuated to the point to where they do not significantly contribute to the overall signal. This could be due to the absorption of the material, or that only a small percentage of the light is actually reflected at each interface. For a wave traveling through a material with an absorption coefficient \(a\), the intensity of the wave will be attenuated by \(e^{-1} \approx 1/3\) after travelling through a distance \(y\) of the material defined as [35]:

\[
y = 1/\alpha(\omega)
\]

The equation above is frequency dependent, meaning that the attenuation will vary across the band for materials without a flat absorption coefficient. As a simple
example, let’s assume a material has a flat absorption coefficient of 20cm$^{-1}$ across the frequency band. The signal would be attenuated by a third after it passes through 500µm of the material. If the material is that same length, then the first satellite pulse to exit the sample (traveling through the material three times total) would be attenuated to $\frac{1}{27}$ of the original incident wave. How much of the signal must be attenuated before it does not contribute to the overall time domain signal will be investigated in chapter 4. However, in the real world the assumption that the above mentioned internal reflections are inconsequential holds for most thick low loss dielectrics; therefore this model can prove to be quite useful [38].

Any measurement performed needs to be calibrated to some known standard if absolute values (instead of relative values) of the real refractive index and absorption are to be determined. To perform the calibration, two measurements are made with a THz TDS system. The first is what is called a “Reference” measurement; which is a measurement performed with the system empty. This can be done in air, or under vacuum; so long as all subsequent measurements are performed under the same conditions. The THz pulse travels over a specified path between the THz source and the detector. The second measurement is made over the same pathway as the reference pulse; however the sample material is placed within the path between the transmitter and detector. This calibration technique works for both transmission and reflection measurements.
Figure 3-1: Reference and sample measurements in a THz TDS system.

To calibrate the measurement, the sample spectrum is divided by the reference spectrum, which in turn eliminates the background from the sample measurement. Also, since the initial conditions for the reference pulse are known, (i.e. performed in vacuum or air), then an absolute value for the sample pulse can be extracted. Also, as discussed in the introduction, the pulses are generated and detected in the time domain; however the calculations are all performed in the frequency domain. To subtract two time domain pulses, very complicated convolution integrals need to be used. Working in the frequency domain allows for simple division of the two frequency spectra (Eqn. 1.1 and Eqn.1.2).

Transforming back and forth between the frequency and time domains is done by using a fast Fourier transform (FFT). This is a discrete Fourier transform method, which is used because the data taken is not continuous. The discrete relationship between the time and frequency domain is given by the following two equations, (the input variables
can be complex). To note, $F(\omega)$ is the complex frequency spectrum, and $f(t)$ is the time domain electric field of the THz pulse.

$$F(\omega) = F_\omega = \sum_{t=0}^{N-1} f_t e^{-i2\pi\omega t} \quad 3.20.$$ 

$$f(t) = f_t = \frac{1}{N} \sum_{\omega=0}^{N-1} F_\omega e^{-i2\pi\omega t} \quad 3.21.$$ 

It is important to note that proper signal processing techniques must be used. The sampling of the FFT must be taken at a power of 2. For example, if 4000 data points were recorded, then either an additional 96 points need to be somehow produced or 1952 points need to be eliminated. The technical computing for this thesis was performed using MATLAB, which has an in-house FFT function that will by default add the additional data points on as zeros to the end of the data array. Unfortunately, this is tampering with the data, since in the time domain all data from the pulse is needed and changing data at the end of the array will corrupt the entire data set.

There is a method for getting around this issue, and it is referred to as “zero-padding.” Essentially, the zeros are added to the front of the data array. This is considered “legal” since technically there should be no time data before the pulse is present. Another benefit to using zero-padding is that it can increase the spectral resolution of the data. The more data points there are to begin with, the more fine the resolution will be once the FFT is completed. This increase in fidelity is due to the increase in the time window of the measurement. Mathematically, the step size of the frequency spectrum is equal to the inverse of the time window. Therefore, the more data points there are, the larger the time
window will be, and the smaller the frequency step size will be. Keep in mind that the time step will be the same regardless of the number of points chosen, just the overall time window will increase with zero-padding. For the measurements performed in conjunction with this thesis, the data sets contained roughly 16500 pts, which is just beyond $2^{14}$. The next power of two is 32768, so instead of zero padding almost twice the number of original data points, the data sets were truncated.

Now, once the reference and sample pulses have been transformed into their frequency domain counterparts, the real and imaginary part of the index of refraction can be calculated. Mathematically, the complex sample spectrum is divided by the complex reference spectrum. Since the time domain signals have been de-convoluted by transforming them into the frequency domain, the part of the sample signal that is related to the environment and the part that is related only to the sample are simply multiplied together. Now, dividing the sample by the reference will therefore cancel out the effect of the environment on the sample pulse, leaving only the effect of the sample on electromagnetic wave.

Going back to equation 3.17 above, and knowing that the complex index of refraction of air/vacuum is simply 1, the ratio of the two fields is given as follows, yielding the complex transmittance function.

$$
\frac{E_s}{E_r} = \frac{e^{(-\omega x n_l/c)} e^{i\omega(t-xn_R/c)}}{e^{i\omega(t-x/c)}} = e^{-(n_l\omega x + i\omega x(n_R+1)/c)}
$$

3.22.
Also to note, the literature surrounding complex refractive index measurements refer to the imaginary part as the absorption [38-39]. The absorption is proportional to the imaginary part by the following relation,

\[ n_I = \alpha(\omega) c / 2\omega \] 3.23.

Substituting the equation 3.23 into equation 3.22 gives the calibrated field equation.

\[ \frac{E_s}{E_r} = e^{-\left(\frac{\alpha x}{2} + \frac{i\omega n_R}{c}\right)} \] 3.24.

The typical measurement performed with a THz TDS is of the THz pulse in the time domain, and then transformed into the frequency domain (via an FFT) to obtain amplitude and phase. The amplitude and phase for the sample and reference pulses can be written respectively as:

\[ \overline{E_s} = |E_{s0}| e^{i\theta_{s0}} \] 3.25.

\[ \overline{E_r} = |E_{r0}| e^{i\theta_{r0}} \] 3.26.

where \(|E_{t0}|\) is the complex amplitude of the field, and \(\theta_{t0}\) is the phase of the field. In a similar fashion, the ratios of these fields can be found by dividing the sample from the reference. The index of refraction and absorption can be found by setting those two equations equal to one another and separating the real and imaginary parts. This method is valid under the assumption that the sample is low-loss and optically thick. Therefore, the following relationships for index of refraction and absorption can be found.
\[ \alpha(\omega) = -\frac{20}{\lambda} \log \left( \frac{|E_{s0}|}{|E_{r0}|} \right) \] 3.27.

\[ n(\omega) = 1 + \frac{c}{\lambda \omega} (\theta_{s0} - \theta_{r0}) \] 3.28.

It is important to note that the value for \( x \) in the above equations is the thickness of the sample. At the beginning of the derivation, the field equation (3.2) had \( x \) in terms of the position of the pulse from some reference (like the transmitter for example). For equations 3.27 and 3.28, the position of the pulse is being defined as the back face of the sample (closest to the detector) in reference to the front face of the sample (i.e. its thickness).

3.3. Ray optics

Another powerful tool often used for optical analysis of systems is ray optics. Ray optics is a geometrical method that uses Snell’s law (among others) to envision how light rays pass through materials, and ignores diffractions. When solving for field equations, one must make use of various integrals, which can make the math fairly difficult. Ray optics utilizes matrix algebra, which is much easier to manipulate, especially when using a computational code such as MATLAB. Another powerful tool of ray optics is the ability to more easily account for interactions at interfaces between two different media. Again, this can be accomplished using Maxwell’s equations; however the math can prove quite difficult.

Whenever light encounters an interface, some of the light is reflected while some of it transmits through. This is always the case, and for the most accurate models these
reflections and transmissions must be taken into account. The transmission and reflection coefficients can be found using the Fresnel equations. The Fresnel equations relate the complex index of refractions of two adjacent layers to what the corresponding reflection and transmission coefficients. In their most general form (not normal incidence), the Fresnel equations are shown to be:

\[
\tilde{t}_{ab}(\omega) = \frac{2\tilde{n}_a(\omega) \cos \theta}{\tilde{n}_a(\omega) \cos \beta + \tilde{n}_b(\omega) \cos \theta} \tag{3.29}
\]

\[
\tilde{r}_{ab}(\omega) = \frac{\tilde{n}_b(\omega) \cos \theta - \tilde{n}_a(\omega) \cos \beta}{\tilde{n}_a(\omega) \cos \beta + \tilde{n}_b(\omega) \cos \theta} \tag{3.30}
\]

where \(a\) refers to the layer the light wave is leaving, \(b\) refers to the layer in which the light ray is entering, \(\tilde{n}_m(\omega)\) is the frequency dependent, complex refractive index of a layer, \(\theta\) is the angle of which the light enters layer \(b\), and \(\beta\) is the angle in which the light is refracted once inside layer \(b\) (based on Snell’s law).

To better understand the geometrical relationships better see Figure 3-2 below (diagram similar to that found in T.D. Dorney, et.al) [52]. It can be seen from the figure that at each interface between the air and the sample, some radiation is lost by either reflecting or transmitting in the backwards dimension. For instance, the first reflection seen, \(r_{01}\), is traveling back towards the source, not towards the direction of propagation. From the figure, \(l\) is the thickness of the sample, \(d\) is the distance that the light travels through the material, and \(m\) is the length through the sample in reference to the incident wave (parallel to \(E_0\)).
Figure 3-2: Ray diagram of sample at random incident angle.

The fields passing through the different layers are defined as before; however now the accommodation has to be made for incident angles other than $0^\circ$. First, the distance that the light travels through the material can be found using geometry.

$$d = \frac{l}{\cos \beta} \quad 3.31.$$ 

Looking at equation 3.16 above the electric field of the propagating wave passing once through the sample is:

$$E_s = E_{\text{const}} e^{(-\frac{i\omega d\tilde{n}}{c})} \quad 3.32.$$
where $E_{\text{const1}}$ is a constant that will be determined shortly. Also to note, the time dependent term $e^{i\omega t}$ is not present. This term is the same in both the reference and the sample measurement. The same method of calibration by dividing the sample spectrum by the reference spectrum will be used, and the terms will cancel themselves out.

If the total distance from the transmit antenna to the receive antenna on the THz TDS system is $x$, then the field equation for the reference is given by:

$$E_{\text{air}} = E_{\text{const2}}e^{(-\frac{i\omega x}{c})} \tag{3.33}$$

where $E_{\text{const2}}$ is another constant to be determined. Now, the field equation for the sample must be extended to include the space before and after the sample. Therefore, the field equations through air with the sample in place are defined as follows.

$$E_{s+\text{air}} = E_{\text{const3}}e^{(-\frac{i\omega (x-m)}{c})} \tag{3.34}$$

To simplify the expressions, and to hold with the convention outlined in T.D. Dorney, *et.al*, the exponential terms will be written as follows [52].

$$p_{\text{sample}} = e^{(-\frac{i\omega d\tilde{n}}{c})}; \quad p_{\text{air}} = e^{(-\frac{i\omega (x-m)}{c})} \tag{3.35}$$

Now, all that needs to be done is to trace out the path that the light follows, adding up the terms as they are encountered. Each time that a ray passes completely through the sample, that field is considered complete, and then the next ray is continued from that point. The extra pulses that are seen are referred to as satellite pulses. They are seen in optically thin samples (keeping note of the fact that whether a sample is optically thin depends heavily on its refractive index). If the sample is too thick, then the time it
takes for the light to bounce around inside the sample and eventually reach the detector is longer than the measurement window or the signal has been completely absorbed by the sample.

As an example, the first ray to pass completely through the sample and then exits is found to be:

\[ E_{first} = E_0 t_{01} p_{sample} t_{10} p_{air} = E_0 t_{01} t_{10} p_{sample} p_{air} \]  \[3.36.\]

while the second field is the same as the first, but takes into account the reflection back into the sample and the reflection back off of the first interface.

\[ E_{second} = E_0 t_{01} p_{sample} r_{10} p_{sample} r_{10} p_{sample} t_{10} p_{air} = E_0 t_{01} t_{10} r_{10}^2 p_{sample}^2 p_{sample} p_{air} \]  \[3.37.\]

A third field equation can be determined following the same procedure.

\[ E_{third} = E_0 t_{01} t_{10} r_{10}^4 p_{sample}^4 p_{sample} p_{air} \]  \[3.38.\]

A simple relation can be shown for an infinite number of internal reflections (see Figure 3-3).

\[ E_{total} = E_0 t_{01} t_{10} p_{sample} p_{air} \left( 1 + \sum_{k=1}^{\infty} \left( r_{10}^2 p_{sample}^2 \right)^k \right) \]  \[3.39.\]

It is important to note that as \( k \) goes to infinity, the measurement (time) window goes to infinity. The number of Fabry-Perot signals (\( k \)) seen depend on not only the length of the delay rail (which is the time window), but also on how much the radiation is lost due to backwards (towards transmitter) reflections and sample loss (\( \alpha \)). The number of Fabry-
Perot signals seen using the Teraview system is generally between 1 and 3. This is discussed further in chapters 4 and 5.

![Figure 3-3: A revised diagram of the multiple pulses that pass through a sample due to internal reflections.](image)

3.4. Reflection losses and satellite pulses

The equation above can be reduced significantly by making several assumptions. First, if the angle of incidence is known to be very close to $0^\circ$, then $\theta = \beta = 0^\circ$. Also, $d = m = l$, which greatly reduces the Fresnel equations, thus making this a simpler problem to solve. These assumptions are only valid if the assumption that the THz radiation is planar is true. However, there are still further simplifications that can be done. If the samples are optically thick (greater than 500 $\mu m$), then the satellite pulses
will never reach the detector in time. Therefore, a simplification can be made to only account for the reflection losses at each interface. Starting with the derived calibrated equation 3.24 above and applying the Fresnel reflection coefficients at the two interfaces, the field ratio can be written as follows.

\[ \frac{E_s}{E_r} = t_{01}t_{10}e^{-\left(\frac{\alpha x}{2} + \frac{i\omega n_2 R}{c}\right)} \]  

\[ t_{01}t_{10}(\omega) = \frac{4 n_1}{(n_1 + 1)^2} \]

Following the same logic as before, and setting this model equal to the magnitude and phase of the measured pulses, corrected index of refraction and absorption equations can be written.

\[ \alpha(\omega) = -\frac{20}{x} \log\left( \frac{|E_{s0}|}{|E_{r0}|} \right) / t_{01}t_{10} \]

\[ n(\omega) = 1 + \frac{c}{x\omega}(\sigma_{s0} - \sigma_{r0}) \]

Notice that the reflection losses only affect the absorption. This is because by definition the absorption is loss; whereas the index of refraction is only related to the phase velocity of the transmitted wave. Therefore, if reflection losses are not accounted for, then the absorption coefficient could be orders of magnitude larger than what the true value is.
3.5. Conclusion

This chapter walked through the development of various electromagnetic models correlating a THz TDS measurement of a flat rectangular sample to the sample’s complex index of refraction. The model continuously evolved to account for the different ways the incident electric field will interact with the sample. First, the simplest model was developed, in which the incident field only interacted with the sample as it propagated through it. Then, the reflection losses at the sample to air interfaces (due to the mismatch between the refractive indices of each material) were taken into account. These reflection losses were determined initially for the low loss sample, where the absorption can be ignored in the Fresnel coefficients.

Next, loss was added in. This made the problem much more complicated because now the field equations could not be solved analytically for the refractive index and absorption. Lastly, a method for accounting for satellite pulses that are seen in optically thin samples was developed. This further complicates things, because now multiple Fresnel reflection and transmission coefficients come into play, all containing both real and imaginary components. These models will now be used to examine measured data. The model will also be validated against measurements provided in the literature, as well as with known samples.
4. Low-loss Optically Thick Sample Assumptions

4.1. Introduction

The first types of samples to be investigated are assumed to be low-loss and optically thick, as defined in chapter 3. Low loss refers to samples with an imaginary component of the refractive index that is much smaller than the real part. When this is true, then only the real part contributes to the Fresnel reflection and transmission coefficients. Optically thick samples are those in which multiple Fabry-Perot reflections do not contribute to the time domain signal. A more detailed description is to follow.

These two assumptions represent the simplest case, but are also relevant to real world problems. Most dielectric materials are low-loss (i.e. high density polyethylene, Teflon, most glasses like Pyrex), making them ideal candidates for this simplified material parameter extraction. The derived equations for the index of refraction and absorption (equations 4.1 and 4.2) for low loss optically thick samples will be used in this chapter. Well known samples that fit within the assumptions listed above will be measured and the extracted values for $n$ and $a$ will be compared to those found in the literature.
\[ \alpha(\omega) = -20 \log \left( \frac{|E_{s0}|}{|E_{r0}|} \frac{t_{01} t_{10}}{t_{02} t_{20}} \right) \]  

\[ n(\omega) = 1 + \frac{c}{\chi \omega} (\sigma_{s0} - \sigma_{r0}) \]

As stated above, with the assumption that the sample is low loss, only the real component of the index of refraction matters in the reflection and transmission coefficients as defined in equations 4.3 and 4.4. Also, only normal incidence will be investigated here, so there will be no angle dependence. The refractive indices \((n_a)\) in the equations below refer to only the real part of the refractive indices:

\[ t_{ab}(\omega) = \frac{2n_a(\omega)}{n_a(\omega) + n_b(\omega)} \]  

\[ r_{ab}(\omega) = \frac{n_b(\omega) - n_a(\omega)}{n_a(\omega) + n_b(\omega)} \]

It is also assumed that the samples are optically thick. As described in chapter 3, an optically thick sample is such that its thickness and refractive index are sufficiently large enough to prevent any multi-pass (also known as satellite) signals from reaching the detector within the time window of the delay rail. This means that even though there might be multiple reflections that eventually make their way through the sample and into the detector, they are either attenuated to the point to where they do not contribute to the overall signal, or lie beyond the measurable time window of the system. In most cases,
the measurement window is large enough to allow for multiple signals to reach the
detector. The real concern is how much they contribute to the overall signal. This will
be investigate in the following section.

4.2. Sample Measurements

Presented below are various material measurements. All measurements were
performed using the Teraview system. The materials presented below are initially
assumed to fit within the assumptions for the model described above. Presented below
are three measured high density polyethylene (HDPE) samples and black high density
polyethylene sample (BHDP). All four samples have a different thickness. The
measured values for $n$ and $a$ are compared to those found in the literature [40,43].

4.2.1. HDPE Sample 1

The first sample that was investigated was a thick piece of high density
polyethylene (HDPE). The sample was 3110 µm thick, and is known to have an index of
refraction of roughly 1.53 from 0.1 to 1 THz, with an absorption coefficient of roughly
0.06 to 0.3 inverse centimeters across the same frequency band [41]. The sample was
measured using the Teraview Spectra 3000 using the internal sample chamber under
normal atmospheric conditions and STP. All samples were measured using this same
device and setup. The length that the delay rail was scanned was 51 mm, corresponding
to a time window of 300 ps. There were a total of 16768 data points taken, which
corresponds to a frequency resolution of roughly 278 GHz. Every sample had a cross-
sectional area larger than the spot size. The spot size of a diffraction limited system is roughly equal to the wavelength of the THz pulse times the $f$ number of the focusing lens [42]. The spot size on the Teraview system was not determined; however an iris with the same dimensions as the spot size (provided by Teraview) was used to verify that all samples were larger than the beam spot (by at least 2 cm). Figure 4-1 below shows the time domain pulses of the HDPE 1 sample and reference measurements. Figure 4-2 is a zoomed in view of just the THz pulses.

![Time Domain Plots of Reference and Sample for 3110 μm thick HDPE](image)

**Figure 4-1:** Measured reference and sample time domain pulses for the HDPE sample.

It can be seen in the figure above that the sample pulse is slightly delayed compared to the reference pulse. Also, the amplitude of the sample pulse is slightly lower than that of the reference pulse. This is expected since the sample should delay the signal (due to the refractive index), as well as absorb some of it as the pulse passes through (due to the absorption and dispersion).
Using the delay above, and the definition of $n$, one can get a good estimate of what the refractive index should be. Again, the definition of $n$ defined in chapter 3 is:

$$n = \frac{c}{v_p}$$  \hspace{1cm} (4.5)

where $c$ is the speed of light in a vacuum and $v_p$ is the phase velocity of the electromagnetic wave traveling through a medium. Also, the velocity of an object traveling at a constant rate can be found by finding the time it takes the object to travel a known distance.

$$v = \frac{\Delta d}{\Delta t}$$  \hspace{1cm} (4.6)

In the above relation, $\Delta d$ would be the change in position of the THz pulse. The change in position in this circumstance would be the thickness of the sample. The THz
pulse traverses that space with and without the sample in place, so \( \Delta d \) is the same for both the reference and sample pulses. Under the assumption that the THz pulse is traveling at a constant rate throughout the material, equation 4.6 would be equal to the phase velocity of the pulse as it passes through the material. Plugging equation 4.6 into 3.9, and getting \( \Delta t \) from the difference in peak positions in Figure 4-2 above, the estimated frequency-averaged index of refraction would be (including units):

\[
n = \frac{c\Delta t}{\Delta d} = \frac{(2.998 \times 10^8 \text{ m/s}) \times (5.50 \pm 0.05 \times 10^{-12} \text{ s})}{(3.110 \pm 0.05) \times 10^{-3} \text{ m}}
\]

\[
n = 1.5 \pm 0.03
\]

This is the same value of 1.53 found in the literature [41]. The error bounds are due to sample thickness measurement error (\( \Delta d \)) and associated error in the time window (\( \Delta t \)). Of course, this estimate is only reasonable for materials whose refractive indices do not vary significantly with frequency. However, this method would still provide a reasonable estimate.

As described in chapter 3, the time domain information is passed through a fast Fourier transform (FFT) to obtain the spectral and phase information. Figure 4-3 and Figure 4-4 below show the frequency spectrum and phase (respectively) for the reference and sample HDPE 1 measurements. In both plots, the measurements are plotted out to 5 THz to show where the signal to noise ratio (SNR) begins. As stated in chapter 2, the Teraview system that was used for this effort has a reported bandwidth of 0.1 – 3 THz; however the noise levels are generally low enough to get usable bandwidth out to 4 THz. This is seen in both plots below. Both the sample and reference spectrums deteriorate into highly oscillatory noise at 4 THz (seen in Figure 4-3). The magnitude of the sample
pulse is slightly lower in amplitude than the reference pulse, which is expected since from equation 4.1, the magnitude uniquely determines the absorption coefficient of the material.

The phase angles in Figure 4-4 begin to exhibit slight oscillations (measurement noise) beginning at 4 THz. The sample phase angle begins to flatten out, showing that the phase information is not reliable past 4 THz. A flat phase angle means that the electromagnetic wave is not oscillating, which is non-physical.

![Frequency Domain Plots of Reference and Sample for 3110 μm thick HDPE](image)

**Figure 4-3:** Measured frequency response of the reference and sample time domain pulses for the HDPE 1 sample.
Figure 4-4: Unwrapped phases of the reference and sample time domain pulses for the HDPE 1 sample.

The phase plot is unwrapped, meaning that the phase is made continuous (instead of sinusoidal) by adding an additional $2\pi$ at each successive phase wrap. The phases at THz frequencies are highly oscillatory, and inverting any equation utilizing the phase would have an infinite number of solutions. Unwrapping the phase presents only one unique solution. The phases presented above go negative, which is simply due to a sign convention on the direction of propagation.

Shown below in Figure 4-5 is the derived refractive index of the HDPE 1 sample, found from equation 4.2.

$$n(\omega) = 1 + \frac{c}{\chi \omega} (\theta_s - \theta_r)$$  \hspace{1cm} 4.8.

The phase angles come from Figure 4-4, $x$ is the sample thickness, $c$ is the speed of light, and $\omega$ is the angular frequency. Notice that the refractive index is fairly flat.
across the frequency band. There is a slight dip from 2 to 2.5 THz, which is mentioned in some journal articles [43]. This dip is due to the fact that the polymer chains in HDPE are tightly packed together and well structured. This provides the material with a crystallinity that exhibits a slight dispersive effect around those particular frequencies [53]. The index of refraction for HDPE is reported to be very flat from 0.1 – 10 THz, which is why it is used for THz optical components such as lenses [43].

![Refractive index of 3110 µm thick HDPE](image)

**Figure 4-5: Index of refraction for HDPE sample.**

As stated above, the absorption is related to the spectral information. The equation relating absorption to the reference and sample spectrums was shown in equation 4.1.

\[
\alpha(\omega) = -\frac{a}{x} \log \left( \frac{|E_{s0}|}{|E_{r0}|} \right)
\] 4.9.
However, equation 4.9 is not entirely correct. When it was first defined in chapter 3, the reflection losses at the sample/air interfaces were not taken into account. As discussed in chapter 3, whenever a light wave is incident on an interface between two different mediums (with different values of $\tilde{n}$), some of the light is reflected at some angle back into the first medium, and some of the light is transmitted into the other medium. For transmission measurements (as was done for this effort), the reflections are essentially a loss, which in turn would increase the calculated value of the absorption coefficient if not taken into account. To account for this loss, the Fresnel transmission coefficient for each interface must be multiplied to the field equation. With the assumption that the material under test is low loss, the real part of $\tilde{n}$ dominates the Fresnel equations. Therefore, the transmission coefficient only affects the magnitude, not the phase angle. The corrected equation for the absorption coefficient is provided below.

$$\alpha(\omega) = -\frac{20}{x} \log \left( \frac{(n(\omega) + 1)^2 |E_\omega|}{4n(\omega)} \right)$$  \hspace{1cm} 4.10.

Shown below in Figure 4-6 and Figure 4-7 is the absorption coefficient of the 3110 µm thick HDPE sample. Shown in both figures is the “thru” calculation, which does not account for reflections between the sample and air interfaces, and the “Fresnel ref. losses”, which does (equation 4.10). Notice that the absorption coefficient is very oscillatory. Any small amount of measurement noise can greatly affect the calculated absorption coefficient. This is due to the fact that the values of the magnitudes of the spectrum are ratios of measured voltages from within the Teraview system. Figure 4-3 above is plotted in logarithmic scale, meaning that the overall trend varies significantly.
across the spectrum, and the only way to view it in a meaningful way is via a log plot. Also in Figure 4-3, the amplitude of the spectrum is decreasing as the frequency increases. This means that the SNR is increasing. This is why the absorption coefficient begins to oscillate vigorously beyond 2 THz. For most low-loss dielectrics however, the absorption coefficient is very flat from 0.1 – 10 THz [43]. Lastly, there are many spikes seen in the absorption plot. These spikes are caused by water vapor’s unique absorption spectrum. Looking back at Figure 4-3, the differences between the amount of absorption due to the water vapor varies between the reference and sample measurements. The peaks at which the absorptions occur are the same; however due to noise in the measurement the actual attenuation is different. This would explain why some of the peaks seen in Figure 4-6 actually go negative. This does not mean that the sample exhibits passive gain, but that the presence of water vapor in the measurement is not entirely accounted for using the calibration technique (dividing the sample by the reference measurements).

![Absorption Coefficient of 3110 μm thick HDPE](image)

**Figure 4-6:** The uncorrected (thru) and corrected (accounting for Fresnel losses at each interface) absorption coefficients of the HDPE sample.
Looking at Figure 4-7, there is an obvious period of oscillation that is seen in both the corrected (Fresnel ref. losses) and uncorrected (thru) absorption coefficients. The period of oscillation is on average 0.0575 THz. When an oscillation like this is seen in the frequency domain, it generally means that there are multiple pulses recorded in the time domain. The extra pulse could possibly be a highly attenuated pulse from multiple reflections within the sample. If this is the case, then the second pulse would have to travel through the sample two additional times compared to the first pulse. If this is the case, then the thickness of the sample can be found by multiplying the period of oscillation above and the phase velocity of the THz pulse as it travels through the sample. This value is calculated to be 3078 µm, which is only 1.1% different than the measured thickness of 3110 µm.

\[
\text{thickness} = \frac{\text{Phase velocity} \ \left(\frac{m}{s}\right)}{2 \ast \text{period (Hz)}} = \frac{c/n}{2 \ast \text{period}} \quad 4.11.
\]

Therefore, the oscillations seen in the absorption coefficient are due to “Fabry-Perot” reflections. This means that this particular sample is not thick enough to attenuate all of the multi-pass signals. However, the amplitude of the oscillations from 0.1-2 THz are 0.4 cm\(^{-1}\); which might be good enough depending on the amount of precision needed. To better quantify a relationship between thickness and multi-pass attenuation, the other HDPE samples will have to be measured and compared.
Figure 4-7: Zoomed in view of the absorption coefficient of the HDPE sample.

There is very little difference between the corrected and uncorrected absorptions in Figure 4-7. This is due to the fact that for this sample, most of the energy is transmitted. To determine how much energy actually propagates through the sample, a value of 1.5 was used for $n$ in equation 4.3. This shows that 96% of the incident radiation will be transmitted through the sample. This leaves only 4% being lost to interface reflections.

4.2.2. Other HDPE Samples

Two other thicknesses of HDPE were measured as well. The samples were 1650 $\mu$m and 19060 $\mu$m. The equations for index of refraction (4.2) and the absorption coefficient with Fresnel losses (4.10) were applied to the measured data for each sample and plotted below. Figure 4-8 is the calculated index of refraction of the two samples.
The calculated refractive index values match the value calculated from the 3110µm sample up to about 2 THz. From 2 – 4 GHz, the thickest sample’s refractive index only slightly dips below the value for 3110 µm (about 3% difference at 4 THz); however the 1650 µm sample has three unphysical discontinuous jumps at 2.2, 2.8, and 3.7 THz, where the phase unwrapping algorithm failed.

**Figure 4-8: Index of refraction for the 1650 and 19060 micron thick HDPE samples.**

Figure 4-9 shows the calculated absorption coefficient for both of the samples. The absorption coefficients plotted in the figure below and the one for the 3110 µm sample plotted in Figure 4-6 trend together. There are oscillations that appear to be thickness dependent. The thinnest sample (1650 µm) has the oscillations with the largest amplitude, while the thickest sample (19060 µm) has the oscillations with the smallest amplitude. This is what would be expected since the contribution from satellite to the overall time domain signal will decrease with sample thickness.
Figure 4-9: Absorption coefficient for the 1650 and 19060 micron thick HDPE samples (including Fresnel reflection losses).

Figure 4-10 below is a zoomed in view of the calculated absorption coefficients for all three HDPE samples. Notice that the period of oscillations tends to decrease with increasing thickness, as would be expected from equation 4.11. The calculated thicknesses are as given in Table 4-1 below. As stated above in the previous section, what is considered optically thick depends on the desired level of accuracy. The 1650 µm sample is optically thin since the amplitudes of the oscillations in the absorption coefficient are almost 1. The only sample to be truly optically thick would be the 19060 µm sample, since the oscillations seen there are losing their periodicity, which means that they are almost entirely in the measurement noise. If a thicker sample could be obtained, the oscillations would most likely be the same as those in the largest sample. Since the largest HDPE sample’s oscillations resembled the noise, the thickness could not be determined, (due to the fact that there was no secondary pulse detected).
### Table 4-1: Measured and calculated thickness for the three HDPE samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Δ Frequency (THz)</th>
<th>Meas. Thickness (µm)</th>
<th>Calc. Thickness (µm)</th>
<th>Percent Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>1650 HDPE</td>
<td>0.0575</td>
<td>1650</td>
<td>1738</td>
<td>5.3%</td>
</tr>
<tr>
<td>3110 HDPE</td>
<td>0.0325</td>
<td>3110</td>
<td>3075</td>
<td>1.3%</td>
</tr>
<tr>
<td>19060 HDPE</td>
<td>0.0058</td>
<td>19060</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

![Absorption Coefficient of HDPE samples](image)

**Figure 4-10:** Zoomed in view of all three HDPE absorption coefficients.

#### 4.2.3. Black HDPE

Lastly, a 12850 µm thick black HDPE sample was measured following the same criteria as described for the HDPE samples. BHDPE has an index of refraction similar to that seen in regular HDPE, about 1.57 from 0.1-10 THz [43]. The absorption is much larger though, ranging from 10-40 cm\(^{-1}\) from 0.1-4 THz, and increasing all the way to 80 cm\(^{-1}\) at 10 THz [43]. The same equations were used to calculate \( n \) and \( \alpha \) that were used for the regular HDPE (equations 4.2 and 4.1 respectively). Shown below in Figure 4-11 and Figure 4-12 are the time and frequency domain plots respectively. The time domain
plot continues past 330 ps; however the sample measurement only contains a single discernible pulse so the plot was truncated for ease of viewing. The frequency domain plot contains some interesting information. The sample spectrum appears to hit the noise floor at 3 THz. This is due to the high absorption values, as well as the large sample thickness.

Figure 4-11: Reference and sample time domain measurements for the 12850 µm thick BHDPE sample.
Figure 4-12: Frequency spectrum for the 12850 µm thick BHDPE sample and reference measurements.

Shown below in Figure 4-13 are the phases of the reference and sample measurements for the 12850 µm thick BHDPE sample. Notice that the sample phase flattens out from 3.4 THz out. There are also small oscillations starting to form at 3 THz onward. This means that the information from about 3 THz onward is too close to the noise floor. This is similar to the noise issues seen in the frequency spectrum. This limits the usable bandwidth to 0.1-3 THz.

Shown in Figure 4-14 is the calculated index of refraction for the 12850 µm thick BHDPE sample. It is fairly flat across the frequency band up to 3 THz, where it starts to drop off. Again, looking at the phase, the measurement hits the noise floor shortly after 3 THz. Nonetheless, the value for n from 0.7 – 3 THz is 1.52, only 3% difference from the value obtained from the literature [43].
Figure 4-13: Phase plots for the reference and sample measurements of the 12850 µm thick BHDPE sample.

Figure 4-14: Refractive index calculations for the 12850µm thick BHDPE sample.

The absorption coefficient for the 12850 µm thick BHDPE sample is shown in Figure 4-15 below. Notice that there are almost no oscillations seen up until about 2.2
THz. After about 2.7 THz the data becomes highly oscillatory, which is expected since the frequency spectrum was approaching the noise floor. The absorption trends as expected, increasing linearly with frequency up to about 2 THz, as was seen in the literature [43]. However, the calculated value for the absorption coefficient from about 1 THz on is slightly higher what was reported in the literature. At 1 THz, the calculated value for $a$ is roughly 10% higher, and increases fairly linearly to about 20% at 2 THz. This is due to the fact that the low loss assumption for the BHDPE sample does not hold. As discussed above, the absorption increases linearly with frequency, so at the lower end of the band (below 1 THz), the assumption is still essentially valid. However, as the frequency and absorption increase, the effect that loss has on the Fresnel coefficients increases. From this, the low-loss assumption is essentially valid up to about 15 cm$^{-1}$.

![Absorption Coefficient of 12850 µm thick Black HDPE](image)

**Figure 4-15:** Absorption coefficient calculation of the 12850 µm thick BHDPE sample.
4.3. Uncertainty Analysis

Some limited uncertainty analysis was performed on the refractive index and absorption coefficient derivations. The only uncertainty that was accounted for was sample thickness. Each sample was measured using a set of Vernier calipers with an associated uncertainty of ±50 µm. This variance was added and subtracted to the nominal thickness value and put into the algorithm. The values obtained are shown as intervals surrounding the nominal derived values. Only the 3110 µm uncertainty is shown below. The variation in the “confidence intervals” would be similar since the samples were similar (in \(n\) and \(\alpha\)). Of course, thinner samples are more affected by the thickness uncertainty than larger samples, but the variations in the 3110 µm sample were minimal, as were the effects in the other two HDPE samples. Therefore, only the 3110 µm uncertainty is shown.

The confidence interval for the refractive index of the 3110 µm HDPE sample is shown in Figure 4-16 below. Only a representative snapshot of the refractive index is shown, not the entire band. This is because the variation is constant over the entire band. This same “snapshot” is shown for all subsequent plots, including the other samples, as well as the confidence intervals for the absorption coefficients. The total variation in \(n\) only ranges about 0.02 across the entire band. Also, a decrease in thickness presents as an increase in \(n\), and vice-versa. This is due to the fact that the algorithm has the same measured phase. If the thickness is smaller, then the apparent increase in phase would present as a larger refractive index. The opposite is true for a thinner sample.
Figure 4-16: Confidence intervals for refractive index based on thickness uncertainty for the 3110 micron thick sample of HDPE.

The variation in absorption coefficient due to sample thickness uncertainty for the 3110 µm HDPE sample is shown in Figure 4-17. The absorption variance was slightly different than the refractive index variance, in that it was a maximum at the peaks of the oscillations. A representative plot of a single peak is shown, but a large number of peaks were inspected across the frequency band and they all had nearly the same variance. The confidence interval spans only about 0.015 cm$^{-1}$. As with the refractive index, a thinner sample (with the same measured spectrum input) would appear to be more absorptive than the thicker sample.

The confidence intervals are fairly tight for both the refractive index and absorption coefficient of the 3110 µm sample. The variation in refractive index due to sample thickness is only ±0.6% across the band, and the maximum variation in
absorption coefficient due to sample thickness (at the peaks) is only ±2.1%. As samples get thinner, this variation will get larger (as will be seen below with the Si wafer).

![Absorption Uncertainty of HDPE Sample Based on Thickness Variations](image)

**Figure 4-17:** Confidence intervals for the absorption coefficient based on thickness uncertainty for the 3110 micron thick sample of HDPE.

The black HDPE was also analyzed using the same criteria. A thickness uncertainty of ±50 µm was run through the algorithms and the same measured phases and spectrums were used. The confidence intervals for the index of refraction and absorption coefficients of the black HDPE sample are shown in the Figure 4-18 and Figure 4-19 respectively. The percent errors for the index of refraction and the absorption coefficient are 0.1% and 0.6% respectively. These are both smaller than the values for the 3110 µm HDPE, due to the fact that the black HDPE is about 4 times thicker than the regular HDPE sample.
Figure 4-18: Confidence intervals for refractive index based on thickness uncertainty for the 12850 micron thick sample of black HDPE.

Figure 4-19: Confidence intervals for the absorption coefficient based on thickness uncertainty for the 12850 micron thick sample of black HDPE.
4.4. Conclusion

Three HDPE samples of various thicknesses were measured and their refractive indices and absorption coefficients were calculated. Also, a black HDPE sample was measured and its refractive index and absorption were calculated. The three HDPE samples had good agreement (within a few percent) of one another in both the index of refraction and absorption coefficient, and also had roughly the same agreement with accepted values in the literature [41]. The initial assumptions made were that the samples were optically thick and low loss. A sample is considered low loss when the imaginary part of the index of refraction (related to absorption) is small enough to ignore that term in the Fresnel reflection and transmission equations (equations 4.4 and 4.3). Optically thick samples are those that any multi-pass internal reflections either do not reach the detector (due to the measurement time window), or are attenuated to the point that they are within the noise floor. From the data presented above, only the thickest HDPE sample and the BHDPE sample could be considered optically thick. The 3110 µm could be considered optically thick, depending on the desired fidelity of the measurement.

However, not all samples will fit within those assumptions. If a sample has an appreciable loss (an absorption coefficient greater than 10 cm\(^{-1}\)) then the loss cannot be ignored in the Fresnel coefficients. As discussed in chapter three, this means that the field equations cannot be inverted to give \(n\) and \(a\). Not to mention that samples that are optically thin will have multiple signals of appreciable amplitudes reach the detector. The following chapter deals with just such a problem.
5. Lossy and Optically Thin Samples

5.1. Introduction

In the previous chapter, low loss and optically thick samples were measured and their respective index of refractions and absorption coefficients were calculated. To reiterate, low loss samples are those with an imaginary index of refraction (related to absorption) that is much smaller than the real part. When this is the case, the contribution of the imaginary part to the Fresnel coefficients (Eqns. 5.1 and 5.2) can be ignored. Optically thick samples are those in which internally reflected time domain pulses do not contribute to the overall measured signal. The number of signals that will make it to the detector is based not only on the thickness, but on the index of refraction of the material as well. From Figure 3-2, \( \theta \) is the incident angle of the radiation, \( \beta \) is the diffracted angle of the radiation inside the sample (as defined by Snell’s law), and \( a \) and \( b \) are the two different materials (\( a \) is air, and \( b \) is the sample).

\[
\begin{align*}
    r_{ab}(\omega) &= \frac{2\tilde{n}_a(\omega) \cos \theta}{\tilde{n}_a(\omega) \cos \beta + \tilde{n}_b(\omega) \cos \theta} \quad 5.1. \\
    r_{ab}(\omega) &= \frac{\tilde{n}_b(\omega) \cos \theta - \tilde{n}_a(\omega) \cos \beta}{\tilde{n}_a(\omega) \cos \beta + \tilde{n}_b(\omega) \cos \theta} \quad 5.2.
\end{align*}
\]
However, the low loss and optically thick assumptions do not hold for all samples. First and foremost, samples could have a loss that will contribute to the Fresnel reflection and transmission coefficients. Also, if the sample is optically thin multiple reflections will be measured in the time domain. Unfortunately, if the sample is lossy or optically thin, then the field equations cannot be solved in closed form for \( n \) and \( \alpha \). This is because the total field is the summation of only a finite number of pulses, not an infinite amount (which can be solved using a geometric series).

\[
E_{\text{total}} = E_0 t_{01} t_{10} p_{\text{sample}} p_{\text{air}} \left\{ \left[ 1 + \sum_{k=1}^{N} (r_{10}^2 p_{\text{sample}})^k \right] \right\} \quad 5.3.
\]

This chapter deals with the problem of an optically thin and lossy sample. A high resistivity Si wafer measuring 500 µm in thickness was measured. The Si wafer’s \( n \) and \( \alpha \) were first determined using the method utilized in chapter 4; however the values for \( n \) and \( \alpha \) did not agree with values found in the literature [45-46]. There are also artifacts that are seen in the plots that are related to the loss and thickness that can be corrected for with the new method outlined.

As stated above, Eq. 5.3 cannot be inverted to solve for \( n \) and \( \alpha \). There are numerical techniques available to invert equations such as 5.3; however none were found capable of providing a solution for \( n \) and \( \alpha \) at each frequency. One such method used was a root finding algorithm known as Newton’s Method [47]. This method sets up a function comparing an initial guess of the unknown variable to the model divided by its derivative (both solved for using the guessed value, see equation 5.4).

\[
x_i = x_{i-1} - \frac{f(x_{i-1})}{f'(x_{i-1})} \quad 5.4.
\]
Newton’s method then finds the zeros of that function by iteration, using the new value for the unknown as the guess for the next iteration. There are three fundamental problems with this method. First, the user has to input a valid initial guess, especially if there are multiple solutions. Second, the method does not handle highly oscillatory inputs (which lead to either multiple solutions or trends towards infinity). To try and get around this hurdle, the unwrapped phase angle of the measured and modeled data were used. Phase angles describe where on the wave an oscillatory function resides at a specific point. Normally, phases are defined on an oscillating interval, such as \([0, 2\pi]\). When a phase is unwrapped, the values run continuously. The unwrapped phase is used primarily for signal processing. Unfortunately, even with an unwrapped phase, the reference and sample spectrums are also too oscillatory.

Another method that can be used is error minimization [48]. Basically, the unknown variable is iterated in the model, and is subtracted from the measurement. The absolute value is taken, and the solution corresponds to the smallest error. This method is also highly susceptible to oscillations in the data and/or model. Another problem with this method is that the error models are single variable. There can be multiple error functions that can be reduced simultaneously; but that only works if the error model being reduced is only dependent on a single variable. For example, in chapter 4 the absorption information was only dependent on the magnitude of the electric field and the refractive index was only dependent on the phase information. For equation 5.3, the magnitude and phase contain both refractive index and absorption information since the Fresnel reflection and transmission coefficients are in terms of both of those variables. This means that an error reduction in one dimension is insufficient for this problem.
There are more advanced optimization techniques that account for covariant error terms. One such method is known as the Nelder-Mead method. The Nelder-Mead method is a non-linear optimization technique that can be applied to twice differentiable unimodal functions [49]. The main drawback to this technique is that it can converge onto another solution. Modern applications of this method constrain the optimizer by applying boundary conditions, and other such constraints. This method was applied to THz TDS of optically thin samples and was shown to be able to converge on a solution for \( n \) and \( a \) that agreed with the values found in literature [50]. However, this method makes use of a confidence interval to bound the optimization. This confidence interval is determined by making several measurements of both the sample and reference pulses at various angles. This is outside of the scope of the problem presented here, which is for single measurements performed at normal incidence. This effort was centered on predicting how a THz time domain pulse would be affected by passing through a flat, homogeneous, and isotropic material. Therefore, since no inversion technique would readily work for this particular problem, the inversion was not pursued.

Even without the inversion available, the model shown in equation 5.3 is still quite useful. If \( n \) and \( a \) of a material are known a priori (across the desired frequency range), then the model can be used to predict what a THz time domain pulse would look like after it passes through a given thickness of the material. Also, if \( n \) and \( a \) are not known then using an error based approach while comparing the predicted and measured time domain pulses will provide an average value of \( n \) and \( a \). These values are the averages across the frequency band. This is similar to the error minimization technique described above, albeit not as robust and therefore solvable. A single value for \( n \) and \( a \)
are used for all frequencies, and then transformed into the time domain. Once in the time domain, the peak amplitudes and positions of the model and measurement are compared.

5.2. Measurements and Data Analysis of High Resistivity Silicon Wafer

A high resistivity (5000 Ω cm) Si wafer was measured using the Teraview TDS internal transmission system described previously. The wafer was 500 µm thick. It was measured under normal temperature and pressure. The wafer was roughly 2 inches in diameter, much larger than the beam spot of the THz radiation. There were 16786 data points taken over a 51 mm long delay rail. This corresponds to a spectral resolution of 2.94 GHz. Figure 5-1 below shows the reference and sample time domain pulses pertaining to the Si wafer.

Seen in Figure 5-2 below, there are three distinguishable pulses in the sample measurement. The first pulse is as expected, attenuated and time delayed, and the other two seem to follow a similar trend being further attenuated and delayed in time. Looking at the extracted spectral magnitude (Figure 5-3), the satellite pulses obviously have an effect. There is a 90 GHz oscillation seen in the sample spectra (see Figure 5-4 for a zoomed in view of the oscillations).
Figure 5-1: Measured reference and sample time domain pulses for the Si wafer.

Figure 5-2: Zoomed in view of the time domain pulses shown in Figure 5-1. The initial pulse, and the two satellite pulse are referenced.
Figure 5-3: Frequency spectrum for the reference and sample measurements for the Si wafer.

Figure 5-4: Zoomed in magnitude of the Si measurements.

These are similar oscillations to those seen in the HDPE samples from the previous chapter. Using the phase velocity of light passing through the material and the period of the oscillations, the thickness of the material can be determined (as shown in chapter 4).
Using Eqn. 4.11, the thickness of the Si wafer is calculated to be 503 µm, within good agreement with the measured thickness of 500 µm.

\[
\text{thickness} = \frac{\text{Phase velocity (m/s)}}{2 \times \text{period (Hz)}} = \frac{c/n}{2 \times \text{period}} \quad \text{(5.5)}
\]

The spectral information shown in Figure 5-3 was used in conjunction with the simple analytic method (no Fabry-Perot reflections accounted for) from chapter 3 for determining the absorption coefficient. The results of that calculation are shown in Figure 5-5. The oscillations in the absorption coefficient are due multiple reflections measured by the detector, exactly like the spectrum. Also note that the average value for the absorption is much higher than what is shown in the literature [45-46]. The absorption coefficient has previously been measured to be an average of 1.8 cm\(^{-1}\) from 0.1-2 THz [46]. The average extracted value using the analytical method is about 10 cm\(^{-1}\) across that same frequency band. This shows that the analytical model for \(\alpha\) is insufficient for optically thin samples.
Figure 5-5: Absorption coefficient for Si wafer using simple extraction routine.

A zoomed in plot of the reference and sample frequency-dependent accumulated phases are shown in Figure 5-6.

Figure 5-6: Reference and sample phase plots for the Si wafer.
Highlighted in red are the small differences between the two phases. These differences correspond to the large discontinuous jumps in the index of refraction calculation seen in Figure 5-7 (at 2.15 and 2.77 THz). These small variations in the phase are due to the satellite pulses seen in Figure 5-1 [52].

![Refractive index of 500 µm thick Si](image)

**Figure 5-7: Refractive index for Si wafer using simple extraction routine.**

As with the absorption coefficient, the analytical model developed in chapter 3 was also used to extract the index of refraction from 0.1 – 4 THz. The index of refraction for a similar high resistivity Si wafer taken from the literature and was reported to be 3.4175 from 0.1 -2 THz, (averaged at all frequencies, but the value only varied by 1%) [46]. The average value of the index of refraction taken from Figure 5-7 is 3.610, in good agreement with the published value. However, the oscillations and discontinuities seen in Figure 5-7 are due to the extraction algorithm not accounting for multi-pass pulses.
To remedy these problems, the field equation developed for lossy, optically thin samples must be used (Eqn. 5.3 below). This equation accounts for multiple pulses, and looking at Figure 5-1 it is clearly seen that there are three pulses. Therefore, the sum in equation 5.3 should be taken twice. Also, the refractive index ($\tilde{n}$) is a function of frequency, but the ($\omega$) was left out to make the equation easier to read.

$$\frac{E_{samp}}{E_{ref}} = \frac{4\tilde{n}}{(\tilde{n} + 1)^2} e^{i\omega(\tilde{n}-1)} \left\{ \left( 1 + \sum_{k=1}^{2} \left( \frac{(\tilde{n} - 1)^2}{(\tilde{n} + 1)^2} e^{2i\omega d}\right)^k \right) \right\}$$

5.6.

As with the previous equation accounting for loss, this function is not analytical. It must be solved by a numerical method. Unfortunately, this equation is highly oscillatory, even using an unwrapped phase. Also, the solutions are not unique, in that the magnitude and phase do not independently define the absorption and refractive index (respectively).

There are methods using a simple error reduction; however these methods do not take into account the covariance between the two unknowns [52]. It is not known if this is a valid method. This function was not inverted to solve for each unknown at each frequency point; however the Si wafer measured has a flat response in refractive index and fairly flat response in absorption [45-46]. This means that the model above can be used to determine a value for $\tilde{n}$ at all frequencies that will match the model to the measurement. The previous figures that show the absorption and refractive index are good starting points. Using the average values as initial inputs to Eqn. 5.3, and iterating over a specified range, the predicted and measured time domain pulses can be aligned, as seen in Figure 5-8 and Figure 5-9 below. The iteration could be performed using a least
squares, or some other error minimization algorithm. For this problem (the Si wafer), it was fairly straightforward and the iteration was performed manually (via inspection). The step-by-step process is as follows:

- Measure each sample (and reference) THz pulse at normal incidence using a THz TDS system.
- Use the simple analytical algorithm developed in chapter three to obtain the initial estimates for $n$ and $\alpha$.
- Using the average value for $n$ and $\alpha$ (averaged at all frequencies within the dynamic range), insert those values into Eqn. 5.3.
- Transform the frequency data back into the time domain and compare measured and predicted THz pulses (compare peak positions and amplitudes).
- Iterate $n$ and $\alpha$ in the frequency domain and perform previous step.
- Continue until the variation between the THz time domain peaks (measured and predicted) is at a minimum.
Figure 5-8: Measured and predicted time domain pulses.

Figure 5-9: Measured and predicted frequency spectrums for the Si wafer.

The predicted and measured pulses line up best with $n = 3.48$ and $a = 1.5$ (average values across the frequency band). This is very close to the reported value of $n = 3.4175$, and $a = 1.8$ [45-46].
5.3. Analysis of Materials From the Literature

To investigate the predictive aspects of this method, multiple sample’s refractive indices and absorption coefficients were collected from various published articles to show what the time domain pulses would look like if they passed through the material. Since $n$ and $\alpha$ are known (taken from the plots provided in the papers), the prediction would be closer to reality than that of the Si wafer (since only average values of $n$ and $\alpha$ were used in that case). To show the robustness of the algorithm, a lossy sample and a dispersive sample were used. The lossy sample is polyimide nylon 6 (PA6). It has a monotonically increasing absorption coefficient of $5 - 80$ cm$^{-1}$ measured from 0.1 to 2.2 THz [53]. Its refractive index is reported to be monotonically decreasing across the same frequency range, running from 1.76 to 1.74 [53]. The plots that were used to obtain these values are shown in Figure 5-10 and Figure 5-10 below [53].

![Figure 5-10: Plots showing the n and a values used for the PA6 sample, (plot includes other polymers as well) [53].](image)

The dispersive sample is cross linked polystyrene (PSX). It is low loss, having an absorption coefficient of 0.1 to $5$ cm$^{-1}$ from 0.1 to 4.2 THz [54]. The refractive index varies considerably over the frequency band, (hence the dispersive quality). It ranges
from 1.592 – 1.584 [54]. The values used (taken from the article) are shown in Figure 5-11 [54].

The same measured reference time domain pulse taken during the Si wafer measurements was used for each hypothetical sample described above (see Figure 5-1 above). With that initial pulse, and the n and α profiles described above, a predicted time domain pulse passing through a particular thickness of each material was calculated. The thicknesses for each material used in the algorithms were the same ones that were reported from each source [53-54]. The PA6 sample was 501μm thick, and the PXS

Figure 5-11: PSX n and α values used from literature. The dark triangles (top lines in both plots) are the PSX values [54].
sample was 1200 µm thick. The PA6 predicted time domain pulse is shown in Figure 5-12, along with the reference pulse.

![Time Domain Plots of Measured Sample and Predicted THz Pulses for 501 µm thick PA6](image)

**Figure 5-12: Predicted time domain pulse for the PA6 sample.**

The predicted pulse is attenuated to about 10% of the original time domain pulse. This large amount of attenuation is due to the high absorption coefficient. The refractive index is not very high, and the sample is only 501 µm thick, so an expected shift of about 1 ps is seen between the peaks. Shown in Figure 5-13 are the reference and predicted spectrums for the PA 6 sample. The spectrums look nearly identical, which is to be expected as the same pulse (and therefore noise) was used to generate both. Also, the absorption is so high, that there are literally no satellite pulses that make it through the material to the detector.
Figure 5-13: Reference and predicted frequency spectrums for the PA6 sample.

The PXS sample is only slightly dispersive (the refractive index varies from 1.592 – 1.584); however the predicted time domain pulse has some chirp. Chirp describes the broadening of a pulse due to a material’s dispersion. A dispersive material (as described in chapter 2), has a refractive index that varies across the frequency band. Since the refractive index varies across the frequency band, different frequencies travel at different velocities through the material. First, this broadens the pulse, yet it also tilts the pulse in one direction or the other (depending on the refractive index profile). Seen below in Figure 5-14, the predicted pulse is starting to broaden, and the shape of the pulse is becoming non-uniform. The full width of the pulse at half maximum (FWHM) of the reference pulse is 0.32 ps, while the FWHM of the PXS pulse is 0.6 ps, almost twice as broad as the reference pulse. Also, the pulse is starting to fall out a Gaussian shape. The peak is starting to shift to the left, making the pulse appear tilted. A more thorough
A discussion of pulse chirping (in reference to ultrafast optics) can be found in the literature. [55]

![Time Domain Plots of Measured Reference and Predicted THz Pulses for 1200 μm thick PXS](image)

**Figure 5-14: Reference and predicted time domain pulses for the PXS sample.**

Lastly, the polyvinylidene fluoride (PVDF) sample was also taken from the literature and run through the predicted model [53]. It was chosen because it has an absorption peak at 1.62 THz. This absorption peak should show some slight oscillating characteristics in the time domain plot due to Fourier analysis. As with the PA6 sample, the complex refractive index information was taken from Figure 5-10. The time domain results are shown in Figure 5-15. Only the predicted sample pulse is shown for ease of viewing. As with the previous predictions, the reference pulse for the Si wafer was used as the measured reference input into the algorithm. The sample is highly absorptive, which is seen from the large amount of attenuation (the amplitude is only about 10% of the original Si wafer reference signal). There are slight oscillations seen across the time window, starting with the pulse at 12 ps, to a minimum at 20 ps, another maximum at
roughly 28 ps, and finally another minimum at 36 ps. This period of 6 ps corresponds to a frequency of 0.6 THz, which is the width of the absorption peak of the PVDF sample.

![Predicted Time Domain Pulse for 511 μm thick PVDF](image)

**Figure 5-15:** PVDF time domain predicted pulse.

![Frequency Domain Plots of Measured Sample and Predicted Spectrum for 511 μm thick PVDF](image)

**Figure 5-16:** PVDF reference and predicted frequency spectrum.
5.4. Uncertainty Analysis

There are many possible sources of uncertainty, including instrument uncertainty, thickness measurement uncertainty, sample placement uncertainty, etc. As stated above, the Teraview Spectra 3000 THz TDS was used for this effort. Their website provides a signal-to-noise ratio that varies across the band, and ranges from 700 to 11000 [56]. The spectral resolution obtained for all of the measurements performed was 2.94 GHz. Looking at some of the finer spectral features (from Figure 5-3), they are on the order of 5 GHz or more, and that is generally oscillations that are attributed to the noise. The important features (such as water vapor lines described in chapter 1) have spectral resolutions on the order of 10’s of GHz, and only occur at specific frequencies. Therefore, it is not believed that the largest contributor to the uncertainty would be the Teraview Spectra system. Also, since measurements were repeatable, and since the samples were all uniform and homogenous, sample placement does not appear to be a very large contributor to the uncertainty. The largest contributor would be the measured thicknesses for the samples. This is simply due to the fact that most of the samples did not have a very uniform thickness. Multiple thickness measurements were performed on all samples, and some varied as much as 100 µm across the surface.

To quantify how error is involved in thickness variations, a simple parametric study was performed. The thickness value for the Si wafer was varied by a certain amount. These new thickness values were used in the predictive algorithm, using the same values for \( n \) and \( \alpha \) that were determined originally. The Si wafer thickness was varied by ±5% and ±10% of the measured value of 500 µm. The 500 µm thickness predicted THz pulse was treated as the measured value, and the absolute difference
between each variation was calculated for both the phase and spectrum (as shown in Eqn. 5.7). The plots of the absolute error in phase are shown in Figure 5-17 and Figure 5-18 below. The plots of the absolute error in magnitude are show in Figure 5-19 through Figure 5-22.

\[
\% \text{ Difference} = \left| \frac{\text{Measured} - \text{Predicted}}{\text{Measured}} \right| \times 100
\]

5.7.

**Figure 5-17:** Absolute phase error due to thickness variation for the Si wafer measurement.
Figure 5-18: Zoomed in view of phase error due to thickness variation for the Si wafer measurement.

Figure 5-19: Absolute spectral error due to ±5% thickness variation for the Si wafer measurement.
Figure 5-20: Zoomed in view of Figure 5-19.

Figure 5-21: Absolute spectral error due to ±10% thickness variation for the Si wafer measurement.
The absolute phase error seems independent of whether it is larger or smaller, just on the actual quantity. The ±5% thickness variations track over the same error. The ±10% thickness variations. The thickness variation error in the spectrum behaves more sporadically. There is a trend between the various thicknesses; however the absolute error appears to be roughly an order of magnitude lower than the signal (see Figure 5-3). The error is highly oscillatory as well, and each set of thickness variations (5 or 10%) seem to have larger packet oscillations.

Lastly, when using the algorithm to find average values for $n$ and $\alpha$ across the frequency band, there is some error involved in finding those average values. For the refractive index, the simple model (described in chapter 4) provides a good starting point in which to start iterating. The absorption coefficient found in the same manner is too high, and it can prove difficult to hone in on the average value. Also, $n$ and $\alpha$ are actually functions of frequency (particularly $\alpha$). Using average values will not perfectly align the
predicted pulses with the measured, so there is already some error before the iterations have begun.

A similar absolute error parametric study was performed using the Si wafer data. The refractive index was varied by 5 and 10% in both the positive and negative directions, as was the absorption coefficient. No covariant terms were investigated (varying both $n$ and $\alpha$ at the same time). Figure 5-23 is of the absolute error of the phase, and Figure 5-24 through Figure 5-27 are of the absolute error of the spectrum for variations in the refractive index in the Si wafer measurements. Unlike the thickness absolute error in phase, the ±5% variation terms do not line up, and neither do the ±10% variation terms. However, there is a point where the phases of the two signals cross. That point corresponds to the turning point in the phase plot below. The spectral refractive index error seems similar to the spectral thickness error. They both appear to follow similar trends, and both appear to be of about the same level.

![Refractive Index Input Variations and Their Effect on the Phase for 500 μm thick Si](image)

**Figure 5-23:** Absolute error in the phase of the Si wafer measurements (iterating over refractive index).
Figure 5-24: Absolute error in the spectrum of the Si wafer measurements (varying the refractive index by ±5%).

Figure 5-25: Zoomed in view of Figure 5-24
Figure 5-26: Absolute error in the spectrum of the Si wafer measurements (varying the refractive index by ±10%).

Figure 5-27: Zoomed in view of Figure 5-26.

The absolute error in the phase of the Si wafer when varying the absorption coefficient is shown in Figure 5-28 (with a zoomed in view in Figure 5-29).
Figure 5-28: Absolute error in phase due to variations in the absorption coefficient for the Si wafer measurements.

Figure 5-29: Zoomed in view of Figure 5-28.

The absolute phase error in this case is much lower than the previous two cases (thickness and $n$). It is also periodic across frequency for all for variations; however it
remains fairly constant (as in a single sine term), its period and amplitude not varying at all.

The absolute spectral error is shown in Figure 5-30 below. This error term is much lower than the previous two spectral errors. Both the thickness and refractive index spectral errors are two orders of magnitude higher than for the absorption error (across the frequency band). This is interesting because for the simple model (chapter 4), the absorption coefficient is uniquely determined by the spectral information. This goes to show how that both the real and imaginary part of the index of refraction can greatly affect the magnitude and phase of the measurement, given a sufficient loss or a thin enough sample. For the zoomed in plot (Figure 5-31), both the 5% variations lie directly on top of one another, as do the 10% variations.

Figure 5-30: Absolute spectral error for the Si wafer measurements (varying the absorption coefficient).
5.5. Conclusion

The predictive model was tested against a measured sample (Si wafer), and two samples borrowed from the literature (PA6 and PXS). Using an average value for $n$ and $\alpha$ (across the entire frequency band) for the Si wafer, the predictive code was able to reproduce the measured time domain pulses to within 6.0% in peak position, and 2.5% in peak amplitude (also averaged from all three pulses). The absolute percent difference was found by taking the difference between the measured and predicted pulse peak positions and amplitudes at each frequency, then dividing that by the measured response and taking the absolute value (as seen in Eqn. 5.7).

There are still variations seen in the Si wafer’s predicted time domain and frequency domain values, but these are most likely due to the fact that $n$ and $\alpha$ are
average values, when in reality they are functions of frequency and do vary across the band [45-46].

However, using a known $n$ and $\alpha$ profile, a prediction of how a time domain pulse will change as it passes through a sample can be made. The model accounts for loss, and for dispersion. This proves to be a novel way of predicting the results of a THz TDS measurement, and can be used to estimate whether a measurement was taken properly.
6. Lossy and Optically Thin Samples

This thesis presented a data analysis and measurement prediction technique for transmission measurements of single slab materials performed with a THz TDS systems. The data analysis included method for determining the refractive index and absorption coefficient for a low-loss, optically thick sample. Also presented was a predictive technique for predetermining what the time domain signal will look like from a lossy optically thin sample. The predictive model was designed to accurately describe real world samples (i.e. lossy, dispersive, etc.). This was achieved by accounting for losses at sample to air interfaces, as well as accounting for multiple internal reflections.

The Teraview Spectra 3000 THz TDS system was used for this effort. Measurements of many materials were performed and used for data analysis and model verification. The materials measured were various thicknesses of HDPE, a single thick piece of black HDPE, and a high resistivity Si wafer. The analytical model (solve for \( n \) and \( \alpha \) from the data) was used on each measured sample. The data was analyzed, and the assumptions of when samples are optically thin and low-loss were determined based on the results.

The Si wafer was also used in the predictive algorithm, showing that, for a given measurement, an average value for \( n \) and \( \alpha \) can be determined. Based on the results of
the analytical model, the values for $n$ and $\alpha$ were iterated and the time domain measured and predicted signals were compared. It was shown that an average value for $n$ and $\alpha$ can be determined that fits the predicted time domain pulse to the measured data. Also, a lossy sample (PA6) and a dispersive sample (PXS) were both investigated using the predicted algorithm. Unlike the Si wafer, these samples were taken from the literature, and their $n$ and $\alpha$ profiles were known across the desired frequency range. These profiles were put into the algorithm, and a predicted time domain pulse was calculated.

All materials investigated for this effort were homogenous and isotropic. There were no composite or structured materials investigated. The models were designed for homogenous samples, and anything other than that would need a revised model. The revised model would have to account for the electromagnetic interactions between the incident fields and the structures. Composite materials that were not homogenous would have to be modeled as they are designed (layered, non-homogenous mixtures, etc.) [57]. If they cannot be modeled, such as a non-homogenous dispersion of particles in a substrate, then approximate methods need to be used [58]. Structured materials such as carbon nanotubes or metamaterials would need to have to have new models as well [59-61]. Also, birefringent materials (such as quartz) were not investigated [62]. In this case, multiple measurements of each sample would have to be performed to characterize the E-field propagation dependent index of refraction.

The models designed were specifically single slab materials (such as high resistivity Si, HDPE, PA6, and PXS), of known thicknesses. The models could be altered to account for multiple layers (such as InMnAs, or InAs) [63]. This will complicate the problem significantly, because there will be multiple Fabry-perot reflections overlapping
one another. Some research groups have presented possible methods for determining the material properties of one layer if the other layer is known (only for a two layer problem) [64]. Of course, as with the inversion techniques described in chapter 5, this problem would have more difficulties, since there would be more possible solutions, and the data would be even more oscillatory. If it was not apparent, this model was designed specifically for complex index of refraction measurements, assuming that the sample thickness was known. It would be trivial to apply the model to a sample with at least one component of the refractive index known and solve for thickness. The model is also structured towards transmission measurements. This can also easily be changed to model reflection measurements by following the same procedure as described in chapter three, but by choosing the appropriate Fresnel coefficients. In the end, the most complicated (and realistic) reflection model would also account for losses at each interface and for multiple reflections within the sample. Lastly, the model was designed for radiation entering at any known angle of incidence; however the measurements were all performed at normal incidence to simplify the code. The incident angle independent functions are presented and can be used instead; however in most cases there is no real benefit to taking off-angle measurements for material characterization purposes for homogenous and isotropic materials, so the simplification is valid in these scenarios. On another note, if a sample’s orientation within the measurements system is one of the unknowns and at least one of the parts of the complex index of refraction is known, then the angle of incidence can be determined.

This thesis centered on terahertz time domain spectroscopy. This is a novel and well understood broadband measurement technique used for determining material
parameters as well as taking THz images of objects. As discussed in chapter one, there are other terahertz measurement methods, including continuous wave (or frequency domain) methods; however the extraction techniques utilized for other methods would differ from THz TDS methods. The main difference between the two different domains is that the frequency domain is steady-state; which means that the transmitted signals are time independent. In the time domain, there is only a single pulse traveling through the material, and there are a finite number of pulses which are detected. The steady-state model (or frequency domain) there is a continuous flow of a specific wavelength of radiation traveling through the material, so the measured transmitted signal is the same at any point in time.

The first extension of this work is to invert the full model to determine the material parameters for each individual frequency. Once a method has been found that effectively solves for the material parameters, this method should be tested by measuring samples with resonances in the absorption spectrum. The next logical extension is updating the model to account for multiple layers. This will encompass accounting for not only the multiple reflections and reflection losses due to each sample, but also the multiple reflections that occur between the different samples. This problem is more difficult, because the differences between which multiple reflection correspond to which sample, as well as which ones correlate to multi-sample reflections must be determined. This is of course dependent on each layer’s thickness and material parameters.

This thesis presented an analytical model for low-loss, optically thick samples that calculates the refractive index and absorption coefficient from measured data. This
model was also shown to provide good initial estimates of $n$ and $\alpha$ for materials that do not fit within the assumptions of low loss or optically thick.

Also presented was a predictive algorithm for predetermining how a THz pulse will be affected when passing through a single rectangular slab of material, given the refractive index and absorption profiles. This includes thick and thin samples (from 500 to 19000 µm in thickness), low loss and lossy samples (absorption ranging from 0.15 to 80 cm$^{-1}$), and moderately dispersive media ($n$ varies by about 10%). This code can be used to compare to measurements and aid in determining the operating status of the THz TDS system being used.
APPENDIX A

MATLAB SCRIPTS

Presented below are the various MATLAB codes that were written in conjunction with this thesis. They were written as independent MATLAB functions. The main functions are written to accept column delimited Excel data files. Each function has its own description, including inputs, outputs, and usage. There are two main functions; all the others are called within these functions. The first function, AnalyticalMethod_FP.m, will solve for \( n \) and \( \alpha \) analytical from an input reference and sample THz TDS measurement. As described above, this method assumes that the sample is low-loss, and there are no satellite pulses detected. The second function is Forward_SingleLayerTHzExt.m, produces the predicted THz TDS pulse based on the sample optical parameters, thickness, and measured reference pulse. The actual predictive algorithm was coded as a separate function called Forward_NMSingleLayer.m. This was done to simplify the code for both writing and troubleshooting purposes. A more detailed description of each of the above functions is presented within each script. There is also included a description of each input and output variable.
The auxiliary functions all perform their specific duties to aid the two previous functions. They are either used by both of the functions, and were written to reduce the complexity of the main functions, or are the actual algorithms used and were separated for ease of viewing. The auxiliary functions are as follows:

- **DCoffset.m**: This function corrects for a DC offset that might occur in the amplitudes of either or both of the reference or sample pulses. This generally occurs when the measurement time window begins to close to the first measured pulse. The offset takes in the amplitude and time information and returns the corrected amplitude and time information for both reference and sample pulses simultaneously.

- **THzFFTnew.m**: This function performs the Fast Fourier transform on the desired time domain pulse. A full description of its inputs and outputs are presented in the script itself.

- **THzIFFT.m**: This function performs the inverse Fast Fourier transform on the desired frequency domain information. A full description of its inputs and outputs are presented in the script itself.

The user will initiate either the AnalyticalMethod_FP. function, or the Forward_SingleLayerTHzExt.m function. All subsequent functions calls performed within these two functions occur independent of the user, and no further user input is needed. Presented below in full are each of the MATLAB functions.
function [n, a, aT2, f] = AnalyticalMethod_FP(DataDir, fid, t,...
    mytitle, varargin)

% AnalyticalMethod_FP - This function takes finds the real and       
%                       imaginary part (absorption coefficient) of the 
%                       refractive index                           
% usage:    [n, a, aT, aT2, f] = AnalyticalMethod_FP(DataDir, fid, t,| 
%                       mytitle, varargin)                       |
% Input Variable:                                                    |
%       DataDir  = The directory that includes the .txt input file   |
% fid      = the .txt file with a single pulse's information   |
%                  contained in 2 columns, (time, amp). The time     |
%                  information can be either be in mm or ps. This is |
%                  the empty cavity measurement.                   |
%       t        = Thickness of the sample (microns)               |
%       mytitle  = The desired title for plotting purposes.        |
% Varagin Inputs:                                                    |
%       plots   = Plot data. 1 = n' and n'' only, 2 = as (1) with FFT|
%                             plot in THz, 3 = as (2) with TD pulse. |
%       saves   = Save data. '.txt' = saves as a .txt file,         |
%                             '.mat' = saves as a .mat file.        |
%                             Leave empty to not save data.         |
% Output Variables:                                                  |
%       n        = The computed real index of refraction.            |
%       a        = The absorption coefficient not accounting for     |
%                  Fresnel reflection losses (cm^-1).                |
%       aT2      = The absorption coefficient accounting for Fresnel|
%                  reflection losses due to both interfaces (cm^-1).  |
%       f        = The frequency information (in THz).               |
% Written by Justin C. Wheatcroft on 2012 May 15                    |
% For the completion of the thesis requirements for the M.S. Physics |
% degree for Wright State University and advisor Dr. Jason Deibel.   |
%--------------------------------------------------------------------

%% Set input variable, read in .txt file.                           
% Append a backslash to DataDir if not already there.               
if ~strcmpi(DataDir(end:end),'\')                                  
    DataDir = [DataDir '\'];                                        
end                                                                  

% Set default values for all variables, query varargin              
format long                                                         
plots = 0; %no plots desired                                        
saves = 'no'; %do not save data                                     
u0 = 4*pi*1e-7; %permeability of freespace (H/m)                   
e0 = 8.854e-12; %permittivity of freespace (F/m)                   
c = 1/sqrt(u0*e0); %speed of light (m/s)                           
n0 = sqrt(u0/e0); %impedance of freespace (ohm)                     
t = t*1e-6;                                                        
for ii = 1:length(varargin)                                         
    arg = cell2mat(varargin(ii));                                    
    if ischar(arg)
switch arg
    case 'plots'
        plots = cell2mat(varargin(ii+1));
    case 'saves'
        saves = cell2mat(varargin(ii+1));
    end
end

if plots == 0
    TDplot = 0;
elseif plots == 1;
    TDplot = 0;
elseif plots == 2;
    TDplot = 1;
elseif plots == 3;
    TDplot = 2;
elseif plots == 4;
    TDplot = 3;
else
    TDplot = 0;
end

%% Read in data and find the usable time range (where the times are equal)
% read sample data from file
pulse = [DataDir fid];
[num,txt,raw] = xlsread(pulse);

% Put "time" data into actual time in seconds
colnum = find(strcmp('Sample Time Domain Signal x axis',txt));
tmp = cell2mat(txt(colnum + 1));
tmp = tmp(end-3:end);
colnum = floor((colnum + 1)/2); %actual column number
if strcmp('(mm)',tmp) == 1 %time data in delay rail length (mm)
timel = 2.*(num(:,colnum)./1000)./c; %put (mm) into (s)
na = find(isnan(timel));
    if isempty(na) == 0
        timel = timel(1:na(1)-1);
    end
else %time data in ps
    timel = num(:,colnum)./1e12; %put (ps) into (s)
    na = find(isnan(timel));
    if isempty(na) == 0
        timel = timel(1:na(1)-1);
    end
end

%Get amplitude data
colnum = find(strcmp('Sample Time Domain Signal',txt));
colnum = floor((colnum + 1)/2);
amp1 = num(:,colnum);
if isempty(na) == 0
    amp1 = amp1(1:na(1)-1);
end

% read reference data from file
%Put "time" data into actual time in seconds
colnum = find(strcmp('Reference Time Domain Signal x axis',txt));
tmp = cell2mat(txt(colnum + 1));
tmp = tmp(end - 3:end);
colnum = floor((colnum + 1)/2); %actual column number
if strcmp('(mm)',tmp) == 1 %time data in delay rail length (mm)
time2 = 2.*(num(:,colnum)./1000)./c; %put (mm) into (s)
na = find(isnan(time2));
if isempty(na) == 0
    time2 = time2(1:na(1)-1);
end
else %time data in ps
    time2 = num(:,colnum)/1e12; %put (ps) into (s)
    na = find(isnan(time2));
    if isempty(na) == 0
        time2 = time2(1:na(1)-1);
    end
end

%Get amplitude data
colnum = find(strcmp('Reference Time Domain Signal',txt));
colnum = floor((colnum + 1)/2);
amp2 = num(:,colnum);
if isempty(na) == 0
    amp2 = amp2(1:na(1)-1);
end
dimtime = time1(5) - time1(4);
tottime = time1(1) - time2(1);
deltime = ceil(tottime/dimtime);
lentime = length(time1);
zeropad = zeros(deltime,1);
amp1 = [zeropad;amp1];
for ii = 1:deltime
    if ii == 1
        zeropad(end) = time1(1) - dimtime;
    else
        zeropad(end - ii + 1) = zeropad(end - ii + 2) - dimtime;
    end
end
time1 = [zeropad;time1];
dimtime = time1(1) - time2(1);
if dimtime > 0
    tmp = time1(1);
tmp = abs(time2 - tmp);
lowbound = find(min(tmp) == tmp);
upbound = length(tmp) - lowbound + 1;
time1 = time1(1:upbound);
amp1 = amp1(1:upbound);
tmp2 = time2(lowbound:length(tmp));
time2 = tmp2;
tmp2 = amp2(lowbound:length(tmp));
amp2 = tmp2;
elseif dimtime < 0
    tmp = time2(1);
tmp = abs(time1 - tmp);
lowbound = find(min(tmp) == tmp);
upbound = length(tmp) - lowbound + 1;
time2 = time2(1:upbound);
amp2 = amp2(1:upbound);
timel = timel(lowbound:length(tmp));
amp1 = amp1(lowbound:length(tmp));
elseif dimtime == 0
end

%% Fix DC offset
[amp1, timel, amp2, time2] = DCoffset(amp1, timel, amp2, time2);

%% Extract data and perform FFT
[~, Y1] = THzFFTnew(timel, amp1, 'plots', TDplot, 'Meas', 'Sample',... 'Zpad', 'no');
[freq Y2] = THzFFTnew(time2, amp2, 'plots', TDplot, 'Meas', 'Reference',... 'Zpad', 'no');
ref = fftshift(Y2);
samp = fftshift(Y1);
npts = length(freq);
var = floor(npts/2)+1:npts;
f = freq(1:length(var));
phiref = unwrap(angle(ref(var)));
phisamp = unwrap(angle(samp(var)));

figure
plot(f,phiref,'r',f,phisamp,'b')
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('Phase (deg)','Fontweight','Bold','Fontsize',12);
title(['Phase plots of ' mytitle],'Fontweight','Bold','Fontsize',16);
legend('Reference','Sample')
xlim([0 4])
grid on

figure
semilogy(f,abs(ref(var)),f,abs(samp(var)));
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('THz Frequency Spectrums (a.u.)','Fontweight','Bold','Fontsize',12);
title(['Frequency Domain Plots of';... '{Reference and Sample for ' mytitle}],... 'Fontweight','Bold','Fontsize',16);
legend('Reference','Sample')
xlim([0 4])
grid on

figure
plot(time2.*1e12,amp2,timel.*1e12,amp1);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitudes (a.u.)','Fontweight','Bold','Fontsize',12);
title(['Time Domain Plots of';... '{Reference and Sample for ' mytitle}],... 'Fontweight','Bold','Fontsize',16);
legend('Reference','Sample')
% xlim([0 5])
grid on

w = 2.*pi.*(f.*1e12); %angular frequency
wv = c./(f.*1e9); %freespace wavelength (m)
k0 = 2*pi./wv; %freespace wavenumber (radians/m)

%% Compute index of refraction and absorption coefficient
n = 1 + (c./(w)).*(-phisamp' + phiref')./t;
T = ((2)./(n+1));
T2 = T.*(((2.*n)./(n+1)));
a = (-2./(t))*log(abs(samp(var))./abs(ref(var)));
aT = (-2./(t))*log(abs(samp(var))./abs(ref(var))).*T';
aT2 = (-2./(t))*log(abs(samp(var))./abs(ref(var))).*T2';

%% Plot if desired

% Real and Imag index of refraction
figure
plot(f,n,'Linewidth',1.5);
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('Refractive Index (n)''','Fontweight','Bold','Fontsize',12);
title([['Refractive index of ' mytitle],...
    'Fontweight','Bold','Fontsize',16]);
xlim([0.1 4]);
ylim([0 4]);
grid on

figure
plot(f,a,f,aT2,'Linewidth',1.5);
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('Absorption Coefficient (1/cm)',...
    'Fontweight','Bold','Fontsize',12);
title([['Absorption Coefficient of ' mytitle],...
    'Fontweight','Bold','Fontsize',16]);
legend('Thru','Fresnel ref. losses','Location','NorthWest');
xlim([0 4]);
ylim([-10 70]); %med HDPE
% ylim([-60 60]); %Si
grid on

%% Data saves
if strcmp(saves,'.txt') == 1
    sample(end-3:end) = [];
    fid = [DataDir sample '_index.txt'];
    fid = fopen(fid,'w');
    for i = 1:1:NFFT/2
        fprintf(fid,'%g %g %g
',freq(i),real(Y(i)),imag(Y(i)));
    end
    fclose(fid);
elseif strcmp(saves,'.mat') == 1
    sample(end-3:end) = [];
    fid = [DataDir sample '_index.mat'];
    save(fid,'freq',Y);
else
    % No data saves
end
return
function [timefp, h2sided, magsamp1,...
    phisamp1, f] = Forward_SingleLayerTHzExt(mytitle, DataDir,...
    fid, t, n, a, varargin)

%-------------------------------------------------------------------------------
% Forward_SingleLayerTHzExt - This functions predicts what the THz-TDS pulse will look like after passing through a known sample.
% usage: [timefp, h2sided, magsamp1, phisamp1, f] = Forward_SingleLayerTHzExt(mytitle, DataDir, fid, t,...
    n, a, varargin)
% Input Variable:
% mytitle = The desired title for plotting purposes.
% DataDir = The directory that includes the .txt input file
% fid = the .txt file with a single pulse's information contained in 2 columns, (time, amp). The time information can be either be in mm or ps. This is the empty cavity measurement.
% t = Thickness of the sample (microns)
% n = The real part of the refractive index. Input can be either a single value, or multiple values as a function of frequency.
% a = The absorption coefficient in terms of inverse cm. Input can be either a single value, or multiple values as a function of frequency.
% Varagin Inputs:
% plots = Plot data. 1 = n' and n" only, 2 = as (1) with FFT plot in THz, 3 = as (2) with TD pulse.
% saves = Save data. '.txt' = saves as a .txt file, '.mat' = saves as a .mat file. Leave empty to not save data.
% Output Variables: (all for the predicted pulse)
% timefp = The time information (in ps).
% h2sided = The amplitude (time domain) information in a.u.
% magsamp1 = The magnitude (frequency domain) information in a.u.
% phisamp1 = The phase (frequency domain) information in a.u.
% f = The frequency information (in THz).
% Written by Justin C. Wheatcroft on 2012 May 15
% For the completion of the thesis requirements for the M.S. Physics degree for Wright State University and advisor Dr. Jason Deibel.
%-------------------------------------------------------------------------------

% Append a backslash to DataDir if not already there.
if ~strcmpi(DataDir(end:end),')
    DataDir = [DataDir '
end

% Set default values for all variables, query varargin
format long
plots = 0; %no plots desired
saves = 'no'; %do not save data
u0 = 4*pi*1e-7; %permeability of freespace (H/m)
e0 = 8.854e-12; %permittivity of freespace (F/m)
c = 1/sqrt(u0*e0); %speed of light (m/s)
n0 = sqrt(u0/e0); % impedance of freespace (ohm)
t = t*1e-6;
for ii = 1:length(varargin)
    arg = cell2mat(varargin(ii));
    if ischar(arg)
        switch arg
            case 'plots'
                plots = cell2mat(varargin(ii+1));
            case 'saves'
                saves = cell2mat(varargin(ii+1));
        end
    end
end

if plots == 0
    TDplot = 0;
elseif plots == 1;
    TDplot = 0;
elseif plots == 2;
    TDplot = 1;
elseif plots == 3;
    TDplot = 2;
elseif plots == 4;
    TDplot = 3;
else
    TDplot = 0;
end

%% Read in data and find the usable time range (where the times are equal)
% read sample data from file
pulse = [DataDir fid];
[num,txt,raw] = xlsread(pulse);

% Put "time" data into actual time in seconds
colnum = find(strcmp('Sample Time Domain Signal x axis',txt));
tmp = cell2mat(txt(colnum + 1));
tmp = tmp(end-3:end);
colnum = floor((colnum + 1)/2); % actual column number
if strcmp('(mm)',tmp) == 1 % time data in delay rail length (mm)
timel = 2.*(num(:,colnum)./1000)./c; % put (mm) into (s)
na = find(isnan(timel));
if isempty(na) == 0
    timel = timel(1:na(1)-1);
end
else % time data in ps
    timel = num(:,colnum)./1e12; % put (ps) into (s)
    na = find(isnan(timel));
    if isempty(na) == 0
        timel = timel(1:na(1)-1);
    end
end

% Get amplitude data
colnum = find(strcmp('Sample Time Domain Signal',txt));
colnum = floor((colnum + 1)/2);
amp1 = num(:,colnum);
if isempty(na) == 0
ampl1 = ampl1(1:na(1)-1);
end

% read reference data from file

% Put "time" data into actual time in seconds
colnum = find(strcmp('Reference Time Domain Signal x axis',txt));
tmp = cell2mat(txt(colnum + 1));
tmp = tmp(end - 3:end);
colnum = floor((colnum + 1)/2); % actual column number
if strcmp('(mm)',tmp) == 1 %time data in delay rail length (mm)
time2 = 2.*(num(:,colnum)./1000)./c; % put (mm) into (s)
na = find(isnan(time2));
if isempty(na) == 0
    time2 = time2(1:na(1)-1);
end
else % time data in ps
    time2 = num(:,colnum)./1e12; % put (ps) into (s)
    na = find(isnan(time2));
    if isempty(na) == 0
        time2 = time2(1:na(1)-1);
    end
end

% Get amplitude data
colnum = find(strcmp('Reference Time Domain Signal',txt));
colnum = floor((colnum + 1)/2);
amp2 = num(:,colnum);
if isempty(na) == 0
    amp2 = amp2(1:na(1)-1);
end

dimtime = time1(1) - time2(1);
if dimtime > 0
    tmp = time1(1);
tmp = abs(time2 - tmp);
lowbound = find(min(tmp) == tmp);
upbound = length(tmp) - lowbound + 1;
time1 = time1(1:upbound);
amp1 = ampl1(1:upbound);
tmp2 = time2(lowbound:length(tmp));
time2 = tmp2;
tmp2 = amp2(lowbound:length(tmp));
amp2 = tmp2;
elseif dimtime < 0
    tmp = time2(1);
tmp = abs(time1 - tmp);
lowbound = find(min(tmp) == tmp);
upbound = length(tmp) - lowbound + 1;
time2 = time2(1:upbound);
amp2 = amp2(1:upbound);
tmp1 = time1(lowbound:length(tmp));
amp1 = ampl1(lowbound:length(tmp));
elseif dimtime == 0
end

%% Fix DC offset
[amp1, time1, amp2, time2] = DCoffset(amp1, time1, amp2, time2);

%% Extract data and perform FFT
[~, Y1] = THzFFTnew(time1, amp1, 'plots', TDplot, 'Meas', 'Sample', ...
    'Zpad', 'no');

[freq Y2] = THzFFTnew(time2, amp2, 'plots', TDplot, 'Meas', ...
    'Reference', ...
    'Zpad', 'no');

ref = fftshift(Y2);
samp = fftshift(Y1);
npts = length(freq);
var = floor(npts/2)+1:npts;
f = freq(1:length(var));
phiref = unwrap(angle(ref(var)));
phisamp = unwrap(angle(samp(var)));
magref = ref(var);
magsamp = samp(var);
npts = length(var);

w = 2.*pi.*(f.*1e12); %angular frequency
wv = c./(f.*1e9); %freespace wavelength (m)
k0 = 2*pi./wv; %freespace wavenumber (radians/m)

%% Begin extraction, loop over all frequencies
[h2sided timefp magsamp1 phisamp1] = Forward_NMSingleLayer(n, a, n1, ...
    t, freq, ...
    ref);
newtime = (time2 - time2(1)).*1e12;

figure
plot(newtime,amp2,'Linewidth',1.5);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitudes (a.u.)','Fontweight','Bold','Fontsize',12);
title('Example Time Domain Reference Signal',...
    'Fontweight','Bold','Fontsize',16);
grid on

figure
plot(newtime,amp2,timefp,h2sided,'Linewidth',1.5);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitudes (a.u.)','Fontweight','Bold','Fontsize',12);
title({'Time Domain Plots of Measured Sample';...
    'and Predicted THz Pulses for ' mytitle},...
    'Fontweight','Bold','Fontsize',16);
legend('Reference','Prediction')
grid on

figure
semilogy(f,abs(magref),f,magsamp1);
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('THz Frequency Spectrums (a.u.)','Fontweight','Bold','Fontsize',12);
title({'Frequency Domain Plots of Measured Sample';...
['and Predicted Spectrum for ' mytitle'],...
'Fontweight','Bold','Fontsize',16);
legend('Reference','Prediction')
xlim([0 5])
grid on

%% Data saves
if strcmp(saves,'.txt') == 1
    sample(end-3:end) = [];
    fid = [DataDir sample '_index.txt'];
    fid = fopen(fid,'w');
    for i = 1:1:NFFT/2
        fprintf(fid,'%g %g %g
',freq(i),real(Y(i)),imag(Y(i)));
    end
    fclose(fid);
elseif strcmp(saves,'.mat') == 1
    sample(end-3:end) = [];
    fid = [DataDir sample '_index.mat'];
    save(fid,'freq','Y');
else
    %No data saves
end
return
function [h2sided, timefp, magsamp, phisamp] = Forward_NMSingleLayer...(n, a, nl, t, freq, ref)

%--------------------------------------------------------------------
% Forward_NMSingleLayer - This is the predicted model. Returns the
%                         predicted information (time and frequency
%                         domain).
% usage:  [h2sided, timefp, magsamp, phisamp] = Forward_NMSingleLayer...(n, a, nl, t, freq, ref);
% Input Variable:
%   n        = The real part of the refractive index. Input can
%                 be either a single value, or multiple values as a
%                 function of frequency.
%   a        = The absorption coefficient in terms of inverse cm.
%                 Input can be either a single value, or multiple
%                 values as a function of frequency.
%   nl       = Refractive index value for layer 1 (air),
%               R + iI.
%   t        = Thickness of unknown layer (m).
%   freq     = Frequency information (THz).
%   ref      = Reference pulse information (in a.u.)
% Output Variables:
%   timefp   = The time information (in ps).
%   h2sided  = The amplitude (time domain) information in a.u.
%   magsamp  = The magnitude (frequency domain) information in
%                 a.u.
%   phisamp  = The phase (frequency domain) information in a.u.
% Written by Justin C. Wheatcroft on 2012 May 20
% For the completion of the thesis requirements for the M.S. Physics
% degree for Wright State University and advisor Dr. Jason Deibel.
%--------------------------------------------------------------------

% Set default values for all variables, query varargin
format long
u0 = 4*pi*1e-7; %permeability of freespace (H/m)
e0 = 8.854e-12; %permittivity of freespace (F/m)
c = 1/sqrt(u0*e0); %speed of light (m/s)
w = 2*pi*(freq*1e12); %angular frequency
w = w';
wv = c./(freq.*1e12); %freespace wavelength (m)
k0 = 2*pi./wv; %freespace wavenumber (radians/m)
n0 = nl; %impedance of freespace (ohm)
a = a.*100;
npts = length(a);
if npts ~= 1
    totpts = length(w);
tmp = sum(a)./npts;
a(end+1:totpts) = tmp;
k = (a.*c)./(2*w);
k(1) = k(2) - (k(3)-k(2));
else
    totpts = length(w);
end
% k = a.*ones(totpts,1);
k = (a.*c)./(2*w);
end
npts = length(n);
if npts ~= 1
    if isnan(n(1))
        n(1) = n(2);
    end
    tmp = sum(n)./npts;
n(end+1:1:totpts) = tmp;
else
    totpts = length(w);
n = n.*ones(totpts,1);
end

%% Combine n
ns = n - 1i.*k;

%% Set up initial Newton's method run
% Set up modeled function
top = 4*n0*ns;
bot = (n0 + ns).^2;
f1 = top./bot;
el = exp(-1.*(1i.*t.*(ns - n0).*w)./c);
FPel = exp(-1.*(1i.*2.*t.*ns.*w)./c);
FPf1 = ((n0 - ns)./(ns + n0)).^2;
FP1 = FPf1.*FPel;
FP2 = (FPf1.^2).*FPel.^2;
FP = 1 + FP1 + FP2;
trans = f1.*e1.*FP;
H = ref.*trans;
npts = length(freq);
var = floor(npts/2)+1:npts;
f = freq(1:length(var));
magsamp = abs(H(var));
phisamp = unwrap(angle(H(var)));

R = magsamp.*cos(phisamp);
Im = magsamp.*sin(phisamp);
fd = R + 1j.*Im;
[h2sided timefp] = THzIFFT(f(2:end), fd(2:end),'Zpad','no');
return
function [amp1, time1, amp2, time2] = DCoffset(amp1, time1, amp2, time2)
% Correct for DC offset in both the signal and reference pulses
% first set up the new time variables (if needed, for each individual
time vector.
timevar1 = zeros(length(time1)-1,1);
for ii = 1:length(time1)-1
    timevar1(ii,1) = time1(ii+1,1) - time1(ii,1);
end
timevar1 = sum(timevar1)/length(timevar1);
timevar2 = zeros(length(time2)-1,1);
for ii = 1:length(time2)-1
    timevar2(ii,1) = time2(ii+1,1) - time2(ii,1);
end
timevar2 = sum(timevar2)/length(timevar2);
%% First offset both amplitude plots by same amount:
tmp = zeros(2,1);
tmp(1,1) = abs(amp1(1));
tmp(2,1) = abs(amp2(1));
tmp = find(min(tmp));
if isempty(tmp) == 1 %both amps start at zero a.u.
    % Do nothing, NO DC offset needed
elseif tmp == 1 %amp2 furthest from zero
    diff = amp1(1);
    amp1 = amp1 - diff;
    amp2 = amp2 - diff;
    if amp2(1) < 0 % first point is neg.
        test = amp2(1) - amp2(2);
        if test > 0 %increasing
            slope = abs(floor(amp2(1)/test));
            rangevar = linspace(0,amp2(1) + test,slope)'; %line to zero
            rng = length(rangevar);
            nptsvar = zeros(rng,1);
            amp2 = [rangevar; amp2];
            timediff = zeros(rng,1);
            for ii = 1:rng;
                if ii == 1
                    timediff(rng,1) = time2(1) - timevar2;
                else
                    timediff(rng - ii + 1,1) = timediff(rng - ii + 2,1) - timevar2;
                end
            end
            time2 = [timediff; time2];
            ampl = [nptsvar; ampl];
            timediff = zeros(rng,1);
            for ii = 1:rng;
                if ii == 1
                    timediff(rng,1) = time1(1) - timevar1;
                else
                    timediff(rng - ii + 1,1) = timediff(rng - ii + 2,1) - timevar1;
                end
            end
        end
    end
timel = [timediff; timel];
elseif test < 0 % decreasing
    deltaslope = linspace(test, -test, 10)';
    amptmp = zeros(length(deltaslope), 1);
    for ii = 1:length(deltaslope)
        if ii == 1
            amptmp(length(deltaslope) - ii + 1, 1) = amp2(1)...
                + deltaslope(ii);
        else
            amptmp(length(deltaslope) - ii + 1, 1) = ...
                amptmp(length(deltaslope) - ii + 2, 1)...
                + deltaslope(ii, 1);
        end
    end
    nptsvar1 = zeros(length(amptmp), 1);
    slope = abs(floor(amptmp(1)/deltaslope(end)));
    rangevar = linspace(0, amptmp(1) + deltaslope(1), slope)';
    nptsvar2 = zeros(length(rangevar), 1);
    nptstot = [nptsvar2; nptsvar1];
    rng = length(nptstot);
    amp2 = [amptmp; amp2]; amp2 = [rangevar; amp2];
    timediff = zeros(rng, 1);
    for ii = 1:rng;
        if ii == 1
            timediff(rng, 1) = time2(1) - timevar2;
        else
            timediff(rng - ii + 1, 1) = timediff(rng...
                - ii + 2, 1) - timevar2;
        end
    end
    time2 = [timediff; time2];
    ampl = [nptstot; ampl1];
    timediff = zeros(rng, 1);
    for ii = 1:rng;
        if ii == 1
            timediff(rng, 1) = timel(1) - timevar1;
        else
            timediff(rng - ii + 1, 1) = timediff(rng...
                - ii + 2, 1) - timevar1;
        end
    end
    time1 = [timediff; timel];
end
elseif amp2(1) > 0 % first point is pos.
    test = amp2(1) - amp2(2);
    if test < 0 % decreasing
        slope = abs(floor(amp2(1)/test));
        rangevar = linspace(0, amp2(1) + test, slope)'; % line to zero
        rng = length(rangevar);
        nptsvar = zeros(rng, 1);
        amp2 = [rangevar; amp2];
        timediff = zeros(rng, 1);
        for ii = 1:rng;
            if ii == 1
                timediff(rng, 1) = time2(1) - timevar2;
            else
                timediff(rng - ii + 1, 1) = timediff(rng...
end

time2 = [timediff; time2];
amp1 = [nptsvar; amp1];
timediff = zeros(rng,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = timel(1) - timevar1;
    else
        timediff(rng - ii + 1,1) = timediff(rng...
            - ii + 2,1) - timevar1;
    end
end
timel = [timediff; timel];
elseif test > 0 %increasing
deltaslope = linspace(test,-test,10)';
amptmp = zeros(length(deltaslope),1);
for ii = 1:length(deltaslope)
    if ii == 1
        amptmp(length(deltaslope) - ii + 1,1) = amp2(1)...
            + deltaslope(ii);
    else
        amptmp(length(deltaslope) - ii + 1,1) = ...
            amptmp(length(deltaslope) - ii + 2,1)... +
            + deltaslope(ii,1);
    end
end
nptsvar1 = zeros(length(amptmp),1);
slope = abs(floor(amptmp(1)/deltaslope(end))); rangevar = linspace(0,amptmp(1) - deltaslope(1),slope)';
nptsvar2 = zeros(length(rangevar),1);
nptstot = [nptsvar2; nptsvar1];
rng = length(nptstot);
apm2 = [amptmp; amp2];
apm2 = [rangevar; amp2];
timediff = zeros(rng,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = time2(1) - timevar2;
    else
        timediff(rng - ii + 1,1) = timediff(rng...
            - ii + 2,1) - timevar2;
    end
end

time2 = [timediff; time2];
amp1 = [nptstot; amp1];
timediff = zeros(rng,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = timel(1) - timevar1;
    else
        timediff(rng - ii + 1,1) = timediff(rng...
            - ii + 2,1) - timevar1;
    end
end
timel = [timediff; timel];
end

elseif tmp == 2 % ampl furthest from zero
    diff = amp2(1);
    amp1 = amp1 - diff;
    amp2 = amp2 - diff;
    if amp1(1) < 0 % first point is neg.
        test = amp1(1) - amp1(2);
    if test > 0 % increasing
        slope = abs(floor(amp1(1)/test));
        rangevar = linspace(0,amp1(1) + test,slope)'; % line to zero
        rng = length(rangevar);
        nptsvar = zeros(rng,1);
        amp1 = [rangevar; amp1];
        timediff = zeros(rng,1);
        for ii = 1:rng;
            if ii == 1
                timediff(rng,1) = time1(1) - timevar1;
            else
                timediff(rng - ii + 1,1) = timediff(rng - ii + 2,1) - timevar1;
            end
        end
        time1 = [timediff; time1];
        amp2 = [nptsvar; amp2];
        timediff = zeros(rng,1);
        for ii = 1:rng;
            if ii == 1
                timediff(rng,1) = time2(1) - timevar2;
            else
                timediff(rng - ii + 1,1) = timediff(rng - ii + 2,1) - timevar2;
            end
        end
        time2 = [timediff; time2];
    elseif test < 0 % decreasing
        deltaslope = linspace(test,-test,10)';
        amptmp = zeros(length(deltaslope),1);
        for ii = 1:length(deltaslope)
            if ii == 1
                amptmp(length(deltaslope) - ii + 1,1) = amp1(1)...
                + deltaslope(ii);
            else
                amptmp(length(deltaslope) - ii + 1,1) = ...
                amptmp(length(deltaslope) - ii + 2,1)...
                + deltaslope(ii,1);
            end
        end
        nptsvar1 = zeros(length(amptmp),1);
        slope = abs(floor(amptmp(1)/deltaslope(end)));
        rangevar = linspace(0,amptmp(1) + deltaslope(1),slope)';
        nptsvar2 = zeros(length(rangevar),1);
        nptstot = [nptsvar2; nptsvar1];
        rng = length(nptstot);
        amp1 = [amptmp; amp1];
        amp1 = [rangevar; amp1];
        timediff = zeros(rng,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = time2(1) - timevar2;
    else
        timediff(rng - ii + 1,1) = timediff(rng... - ii + 2,1) - timevar2;
    end
end
time1 = [timediff; time1];
amp2 = [nptstot; amp2];
timediff = zeros(rng,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = time2(1) - timevar1;
    else
        timediff(rng - ii + 1,1) = timediff(rng... - ii + 2,1) - timevar1;
    end
end
time2 = [timediff; time2];
end
elseif amp1(1) > 0 % first point is pos.
test = amp1(1) - amp1(2);
if test < 0 %decreasing
    slope = abs(floor(amp1(1)/test));
    rangevar = linspace(0,amp1(1) + test,slope)'; %line to zero
    rng = length(rangevar);
    nptsvar = zeros(rng,1);
    amp1 = [rangevar; amp1];
    timediff = zeros(rng,1);
    for ii = 1:rng;
        if ii == 1
            timediff(rng,1) = time1(1) - timevar1;
        else
            timediff(rng - ii + 1,1) = timediff(rng... - ii + 2,1) - timevar1;
        end
    end
    time1 = [timediff; time1];
    amp2 = [nptsvar; amp2];
    timediff = zeros(rng,1);
    for ii = 1:rng;
        if ii == 1
            timediff(rng,1) = time2(1) - timevar2;
        else
            timediff(rng - ii + 1,1) = timediff(rng... - ii + 2,1) - timevar2;
        end
    end
    time2 = [timediff; time2];
elseif test > 0 %increasing
    deltaslope = linespace(test,-test,10)';
    amptmp = zeros(length(deltaslope),1);
    for ii = 1:length(deltaslope)
        if ii == 1
            amptmp(length(deltaslope) - ii + 1,1) = amp1(1)... + deltaslope(ii);
else
    amptmp(length(deltaslope) - ii + 1,1) = ...
    amptmp(length(deltaslope) - ii + 2,1)...
        + deltaslope(ii,1);
end
end
nptsvar1 = zeros(length(amptmp),1);
slope = abs(floor(amptmp(1)/deltaslope(end)));
rangevar = linspace(0,amptmp(1) + deltaslope(1),slope)';
nptsvar2 = zeros(length(rangevar),1);
nptstot = [nptsvar2; nptsvar1];
rng = length(nptstot);
ampl = [amptmp; ampl];
ampl = [rangevar; ampl];
timediff = zeros(ring,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = time1(1) - timevar1;
    else
        timediff(rng - ii + 1,1) = timediff(rng...
            - ii + 2,1) - timevar1;
    end
end
time1 = [timediff; time1];
amp2 = [nptstot; amp2];
timediff = zeros(ring,1);
for ii = 1:rng;
    if ii == 1
        timediff(rng,1) = time2(1) - timevar2;
    else
        timediff(rng - ii + 1,1) = timediff(rng...
            - ii + 2,1) - timevar2;
    end
end
time2 = [timediff; time2];
end
function [freq Y] = THzFFTnew(time, amp, varargin)
%
%--------------------------------------------------------------------
% THzFFT - This function takes a time domain THz pulse and returns
% the FFT and frequency information.
% usage: [freq Y] = THzFFT(DataDir, fid, varargin)
%
% Input Variable:
% DataDir = The directory that includes the data input file
% fid = the .csv file with a single pulse's information
% The time information can be either be in mm or ps.
% varargin = Variable argument that takes a user input and
% performs a specific function. Input example:
% [freq Y] = THzFFT(DataDir, fid, 'plots',2);

Varargin Inputs:
plots = Plot data. 1 = FFT only, 2 = FFT and TD pulse,
3 = FFT, TD, and TD with zero padding.
saves = Save data. '.txt' = saves as a .txt file,
'.mat' = saves as a .mat file.
Zpad = User defined zero padding. 'yes' = uses the next
power of 2 for zero padding. 'no' = uses previous
power of 2, no zero padding. If left undefined the
user will be prompted in the main window with zero
padding options.
bounds = User defined bound for the frequency domain plot.
Input as a single number for the maximum THz
frequency displayed on the x-axis.
Meas = Determine whether the 'Signal' or 'Reference' data
is desired, (input variable as above).
'Reference' will be used if left empty.

Output Variables:
freq = The frequency domain information.
Y = The complex information derived from the fft.m
function. Saved as real and imaginary.

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--------------------------------------------------------------------

%% Set input variable, read in .txt file.

% Set default values for all variables, query varargin
format long
plots = 0; %no plots desired
saves = 'no'; %do not save data
Zpad = 'query'; %query the user in the command window
bounds = 4; %set intial bounds for the FFT plot x-axis to 4 THz
Meas = 'Reference';

for ii = 1:length(varargin)
    arg = cell2mat(varargin(ii));
    if ischar(arg)
        switch arg
            case 'plots'
                plots = cell2mat(varargin(ii+1));
case 'saves'
saves = cell2mat(varargin(ii+1));
case 'Zpad'
Zpad = cell2mat(varargin(ii+1));
case 'bound'
bound = cell2mat(varargin(ii+1));
case 'Meas'
Meas = cell2mat(varargin(ii+1));
end
end
end

%% Determine zero padding and set up frequency domain
npts = length(time);
NFFT = 2^nextpow2(npts);
switch Zpad
    case 'query'
disp(['The total number of points is ' mat2str(npts) '.']);
disp(['The next power of 2 is ' mat2str(NFFT) '.']);
disp('Would you like to zero pad the data?');
tmp = input('1 = Yes, 2 = No : ');
    if tmp == 2
        NFFT = npts;
        htitle = 'without zero padding';
    else
        htitle = 'with zero padding';
    end
    case 'yes'
    %NFFT is already set
    htitle = 'with zero padding';
    case 'no'
        NFFT = npts;
        htitle = 'without zero padding';
end
numz = NFFT - npts; %length of zero padding

if isequal(numz,0) == 0 %if zero padding the data, then...
zpad = zeros(numz,1);
newamp = [zpad; amp]; %updated amp with zpad
tn = zeros(length(time)-1,1);
for ii = 1:length(time)-1
    tn(ii,1) = time(ii+1) - time(ii);
end
tn = sum(tn)/length(tn);
t0 = time(1); %initial time before zpad
for ii = 1:numz;
    zpad(numz - (ii - 1),1) = t0 - ii*tn;
end
newtime = [zpad; time]; %updated time with zpad
else %if not zero padding the data
    newamp = amp;
    newtime = time;
end

%% Perform FFT and determine frequency range
Y = fft(newamp,NFFT);
Yplot = Y(1:floor(NFFT/2));
twindow = newtime(end) - newtime(1); %total time
freq = ((1/twindow).*(0:1:NFFT-1))*1e-12;
fplot = freq(1:floor(NFFT/2))/1;

%% Plot if desired

%Frequency domain
if isequal(plots,0) == 0;
tmp = 'FFT of the THz TD Pulse ';
htitle = [tmp htitle];
figure
semilogy(fplot,abs(Yplot),'Linewidth',1.5);
xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
ylabel('Power','Fontweight','Bold','Fontsize',12);
title(htitle,'Fontweight','Bold','Fontsize',16);
xlim([0.1 bound]);
grid on
end

% Time domain pulse without zpad
if plots == 2 || plots == 3;
figure
plot(time*1e12,amp,'Linewidth',1.5);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitude (V/m)','Fontweight','Bold','Fontsize',12);
title('TD THz Pulse','Fontweight','Bold','Fontsize',16);
grid on
end

% Time domain pulse with zpad
if plots == 3;
figure
plot(newtime*1e12,newamp,'Linewidth',1.5);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitude (V/m)','Fontweight','Bold','Fontsize',12);
title('TD THz Pulse with Zero Padding',...
'Fontweight','Bold','Fontsize',16);
grid on
end

%% Data saves
if strcmp(saves,'.txt') == 1
fid(end-3:end) = []; 
 fid = [DataDir fid '_FFT.txt'];
 fid = fopen(fid,'w');
 for i = 1:1:NFFT/2
 fprintf(fid,'%g %g %g
',freq(i),real(Y(i)),imag(Y(i)));
 end
fclose(fid);
elseif strcmp(saves,'.mat') == 1
fid(end-3:end) = []; 
 fid = [DataDir fid '_FFT.mat'];
 save(fid,'freq','Y');
else
 %No data saves
 end
return
function [h2sided time] = THzIFFT(freq, Y, varargin)
% This function takes the single sided frequency domain THz data and returns the time and amplitude information.
% usage: [h2sided time] = THzIFFT(freq, Y, varargin)

% Input Variable:
% freq   = The frequency information in (1,N) format
% Y      = The power information as derived from the THzFFT.m function. This is the single-sided information, and must be the same number of points as freq.
% varargin = Variable argument that takes a user input and performs a specific function. Input example: [h2sided time] = THzIFFT(freq, Y, 'plots',2);

% Varargin Inputs:
% plots   = Plot data. 1 = IFFT only, 2 = IFFT and FFT
% saves   = Save data. '.txt' = saves as a .txt file, '.mat' = saves as a .mat file.
% Zpad    = User defined zero padding. 'yes' = uses the next power of 2 for zero padding. 'no' = uses previous power of 2, no zero padding. If left undefined the user will be propted in the main window with zero padding options.

% Output Variables:
% h2sided = The double-sided amplitude information.
% time    = The time information (ps).

% Written by Justin C. Wheatcroft on 2012 May 20
% For the completion of the thesis requirements for the M.S. Physics degree for Wright State University and advisor Dr. Jason Deibel.

%% Set default values for all variables, query varargin, set up Zpad format long
plots = 0; %no plots desired
saves = 'no'; %do not save data
Zpad = 'query'; %query the user in the command window
zero = 0; %no FFT zero-padding removed from plot
for ii = 1:length(varargin)
    arg = cell2mat(varargin(ii));
    if ischar(arg)
        switch arg
            case 'plots'
                plots = cell2mat(varargin(ii+1));
            case 'saves'
                saves = cell2mat(varargin(ii+1));
            case 'Zpad'
                Zpad = cell2mat(varargin(ii+1));
            case 'zero'
                zero = cell2mat(varargin(ii+1));
        end
    end
end
npts = length(freq);
NIFFT = 2^nextpow2(npts);

switch Zpad
  case 'query'
    disp(['The total number of points is ' mat2str(npts) '.']);
    disp(['The next power of 2 is ' mat2str(NIFFT) '.']);
    disp('Would you like to zero pad the data?');
    tmp = input('1 = Yes, 2 = No : ');
    if tmp == 2
      NIFFT = npts;
      htitle = 'without zero padding';
    else
      htitle = 'with zero padding';
    end
  case 'yes'
    % NIFFT is already set
    htitle = 'with zero padding';
  case 'no'
    NIFFT = npts;
    htitle = 'without zero padding';
  end

numz = NIFFT - npts; % length of zero padding

if isequal(numz,0) == 0 % if zero padding the data, then...
  zpad = zeros(numz,1);
  newY = [Y; zpad]; % updated amp with zpad
  fn = freq(10) - freq(9); % time step
  f0 = freq(end); % initial time before zpad
  for ii = 1:numz;
    zpad(ii,1) = f0 - ii*fn;
  end
  newfreq = [freq; zpad]; % updated time with zpad
else % if not zero padding the data
  newY = Y;
  newfreq = freq;
end

% Perform IFFT and determine time range

fn = newfreq(10) - newfreq(9); % frequency step
per = 1/fn; % total time
tn = per/NIFFT; % time step
time = (0:tn:per-tn)'; % time interval from 0 ps

h1shifted = ifft(newY,NIFFT);
h2sided = cos(2*pi*newfreq(1)*time).*real(h1shifted) - ...
          sin(2*pi*freq(1)*time).*imag(h1shifted);

% Plot if desired
% Frequency domain
if isequal(plots,0) == 0;
  tmp = 'IFFT of the THz spectra ';
  htitle = [tmp htitle];
  figure
  plot(time,h2sided,'Linewidth',1.5);
xlabel('Time (ps)','Fontweight','Bold','Fontsize',12);
ylabel('Amplitude','Fontweight','Bold','Fontsize',12);
title('htitle','Fontweight','Bold','Fontsize',16);
grid on
end

% Original Frequency domain plot
if plots == 2;
    figure
    semilogy(freq,abs(Y),'Linewidth',1.5);
    xlabel('Frequency (THz)','Fontweight','Bold','Fontsize',12);
    ylabel('Power','Fontweight','Bold','Fontsize',12);
    title('Frequency Spectrum','Fontweight','Bold','Fontsize',16);
    xlim([0.1 4]);
    grid on
end

%% Data saves
if strcmp(saves,'.txt') == 1
    fid = ['THzIFFTdata' num2str(length(dir)) num2str(randi(13)) '.txt'];
    fid = [pwd '\' fid];
    fid = fopen(fid,'w');
    for ii = 1:1:NFFT
        fprintf(fid,'%g %g
',time(ii),h2sided(ii));
    end
    fclose(fid);
elseif strcmp(saves,'.mat') == 1
    fid = ['THzIFFTdata' num2str(length(dir)) num2str(randi(13)) '.mat'];
    fid = [pwd '\' fid];
    save(fid,'time','h2sided');
else
    %No data saves
end
return
REFERENCES


[43] P.D. Cunningham, et. al, “Broadband terahertz characterization of the refractive index and absorption
of some important polymeric and organic electro-optic materials,” J. Appl. Phys. 109, 043505 (2011)


