

Three Dimensional T-Ray Inspection Systems

by

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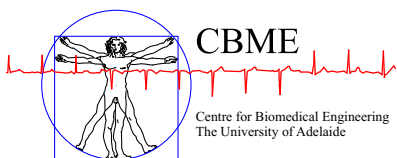
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Abstract

Pulsed terahertz (THz) systems are an emergent technology, finding diverse applications as they approach maturity. From their birth in the late 1980's to the wealth of alternate sources and imaging modalities now available, the rise has been fuelled by the expectation that this will prove a world changing technology. This Thesis takes an application focused approach and seeks to provide enabling systems and algorithms for the development of *functional* imaging systems with broad potential application in security inspection, non-destructive testing and biomedical imaging.

Three dimensional pulsed THz imaging systems were first introduced in 1996 using a reflection-mode ultrasound-like configuration. This Thesis builds upon this former work by focusing on *transmission* mode tomography systems using pulsed THz radiation. Several novel 3D imaging modalities are introduced. The hardware architectures, based on optoelectronic generation and detection of THz radiation are described. Approximations to the wave equation are derived, allowing linear reconstruction algorithms to recover 3D structural information from the transmitted THz field. Finally the systems are demonstrated and the achievable resolution and image quality are investigated. Three imaging architectures are developed herein:

1. T-ray holography allows the 3D distribution of point scatters to be resolved based on a single projection image utilising a novel reconstruction algorithm based on the windowed Fourier transform and back-propagation of the Fresnel-Kirchhoff diffraction equation.
2. T-ray diffraction tomography utilises the diffracted THz field to allow a Helmholtz equation based, frequency-dependent reconstruction to be performed and the THz spectrum at each pixel to be calculated.
3. T-ray Computed Tomography (CT) uses analogous techniques to X-ray CT, based on the Radon transform, to provide 3D T-ray reconstructions of unprecedented fidelity.

These techniques have important applications in material identification, which is investigated in the second part of this Thesis.

Pulsed THz spectroscopy has been widely acclaimed for its potential to identify different materials based on their spectral properties. The second part of this Thesis presents algorithms towards this goal. Three case studies are performed focusing on biomaterial classification, anthrax detection and *in vitro* osteosarcoma cell differentiation. A classification framework is developed to process the THz spectral data and identify specific materials. A linear filter model is introduced to describe the system response of different materials, and the filter taps are utilised for feature extraction. This technique is demonstrated for biomaterial and anthrax classification. For cell differentiation a genetic algorithm is used to select deconvolved frequency components to train a classifier. In each case a high classification accuracy is demonstrated, highlighting the promise and potential of three dimensional T-ray inspection systems.

Statement of Originality

This work contains no material that has been accepted for the award of any other degree or diploma in any university or other tertiary institution and, to the best of my knowledge and belief, contains no material previously published written by another person, except where due reference has been made in the text.

I give consent to this copy of the thesis, when deposited in the University Library, being available for loan, photocopying and dissemination through the digital thesis collection.

A handwritten signature in black ink, appearing to read 'B. Ferguson'.

29th December, 2004

Signed

Date

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A great number of people have collaborated to make this Ph.D. an exceptionally rewarding and memorable experience. I extend my sincerest thanks to my family, friends, colleagues and supervisors for their support and encouragement.

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I had the pleasure of working with one of the true pioneers of THz imaging, Professor X.-C. Zhang (Rensselaer Polytechnic Institute, USA). I hold him in the highest esteem for captivating me with his vision of the potential of THz research and for his inspiration and guidance.

While a Ph.D. is, by nature, a solitary experience, I have benefitted greatly from interaction with colleagues at the University of Adelaide and at Rensselaer Polytechnic Institute. I wish to acknowledge Dr Samuel Mickan, Dr Greg Harmer, Leonard Hall, Hua Zhong, Haibo Liu and Jingqun Xi. A special debt of gratitude is also owed to Dr Shaohong Wang from Rensselaer Polytechnic Institute. Much of the work in this Thesis is a result of our fruitful collaboration.

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I thank my parents for their love and for teaching me that “... *the LORD gives wisdom, from His mouth come knowledge and understanding.*” – Proverbs 2:6. I also thank the rest of my family: Daniel, Cameron, Mark, Amanda and Rebecca, for memories and support.

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"Well, in our country," said Alice, still panting a little, "you'd generally get to somewhere else – if you ran very fast for a long time, as we've been doing."

"A slow sort of country!" said the Queen. "Now here, you see, it takes all the running you can do, to keep in the same place. If you want to get somewhere else, you must run at least twice as fast as that."

- Lewis Carroll (Carroll 1936)

"There are only two ways to live your life. One is as though nothing is a miracle. The other is as though everything is a miracle."

- Albert Einstein

Thesis Conventions

Typesetting. This Thesis is typeset using the L^AT_EX2e software. Processed plots and images were generated using Matlab 6.1 (Mathworks Inc.). CorelDRAW 8.4 (Corel Corporation) was used to produce schematic diagrams and other drawings. Pixotec Slicer Dicer (Pixotec Inc.) was used to generate 3D rendered images.

Spelling. Australian English spelling has been adopted throughout, as defined by the Macquarie English Dictionary (A. Delbridge, Ed., Macquarie Library, North Ryde, NSW, Australia, 2001). Where more than one spelling variant is permitted such as 'biassing' or 'biasing' and 'infra-red' or 'infrared' the option with the fewest characters has been chosen.

Referencing. The Harvard style is used for referencing and citation in this Thesis.

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Introduction and Motivation

THREE dimensional pulsed terahertz (THz) imaging systems were first demonstrated in 1996. Of late this field is undergoing something of a renaissance as THz sources and detectors have developed to a point where high signal to noise ratio and reasonable acquisition rates are possible. One key objective is to combine three dimensional imaging with spectroscopic information capture.

A further challenge in THz systems is that of devising signal processing methods to derive information from the THz spectroscopic data. In particular the problem of identifying specific materials based on the THz response has broad reaching applications. Most molecules (particularly solids) have very complicated THz absorption spectra with a multitude of absorption lines subject to thermal broadening at room temperature. This reduces the applicability of traditional spectral analysis methods at room temperature and motivates the current work.

This Thesis brings together the fields of three dimensional imaging and spectroscopic analysis. It concentrates on hardware architectures and software algorithms towards the goal of fully automated, three dimensional THz inspection systems.

1.1 Introduction

This Chapter introduces the field of THz (T-ray) spectroscopy and discusses the motivation for this work towards three dimensional (3D) THz inspection systems. It provides a roadmap for the Thesis and a concise summary of the novel contributions represented by this work.

1.1.1 THz Radiation

The THz region of the electromagnetic spectrum has proven to be one of the most elusive. THz radiation is loosely defined¹ by the frequency range of 0.1 to 10 THz (where 1 THz is 10^{12} cycles/second). Situated between infrared (IR) light and microwave radiation (see Fig. 1.1), it is somewhat resistant to the techniques commonly employed in these well-established, neighbouring bands. High atmospheric absorption constrained early interest and funding in THz science – historically the major domain of THz spectroscopy has been in spectral characterisation of the rotational and vibrational resonances, and thermal emission lines of simple molecules by chemists and astronomers. Since the 1980s, we have seen a revolution in THz systems, as advanced materials research provided new and higher power sources and the potential for advanced physics research and commercial applications has been demonstrated. It is an extremely attractive research field with interest from sectors as diverse as the semiconductor, medical, manufacturing, aerospace, and defence industries. A number of recent major technical advances have greatly extended the potential and profile of THz systems. These advances include the development of a quantum cascade THz laser (Köhler et al. 2002), the demonstration of THz detection of single base-pair differences in femtomol concentrations of DNA (Huber et al. 2001), and the investigation of the evolution of multi-particle charge interactions with THz spectroscopy (Cole et al. 2001a).

¹Although this is a common definition in the literature, a number of authors define 0.3 to 30 THz as the T-ray band. A consensus has not yet been reached. We have adopted 0.1 to 10 THz as it closely corresponds to the traditional ‘terahertz gap’ region.

1.2 Background

1.2.1 The Electromagnetic Spectrum

Electromagnetic radiation is propagated by photons. Each photon has an associated energy that determines both its frequency and wavelength. At low frequencies (radio frequency, RF, and below) the photons have very small energies, and cannot be measured individually. Radio waves consist of large numbers of photons, which result in coherent, polarised electric and magnetic fields. These fields can be measured by the voltage they induce in an antenna, and it is appropriate to discuss this electromagnetic radiation in terms of its wave nature.

At higher frequencies (infrared and above) the fields oscillate too quickly to be measured conventionally. Instead individual photons have sufficient energy to be measured, for example using photovoltaic devices, or photoreceptor molecules in our eyes. Since individual photons may be detected, particle terminology is often used to describe this radiation.

The THz frequency band lies on the border of these two regimes as illustrated in Fig. 1.1.

1.2.2 THz Spectroscopy Systems

THz spectroscopy allows a material's far-infrared optical properties to be determined as a function of frequency. This information can yield insight into material characteristics for a wide range of applications. A number of different methods exist for performing THz spectroscopy. Fourier transform spectroscopy (FTS) is perhaps the most common technique used for studying molecular resonances. It has the advantage of an extremely wide bandwidth, enabling material characterisation from THz frequencies to well into the infrared. In FTS, the sample is illuminated with a broadband thermal source such as an arc lamp or a silicon carbide (SiC) globar. The sample is placed in an optical interferometer system and the path length of one of the interferometer arms is scanned. A direct detector such as a helium cooled bolometer is used to detect the interferometric response. The Fourier transform of the signal then yields the power spectral density of the sample. One disadvantage of FTS is its limited spectral resolution. Much higher resolution spectral measurements may be made using a narrowband system utilising a tunable THz source or detector. In these systems the source

1.2 Background

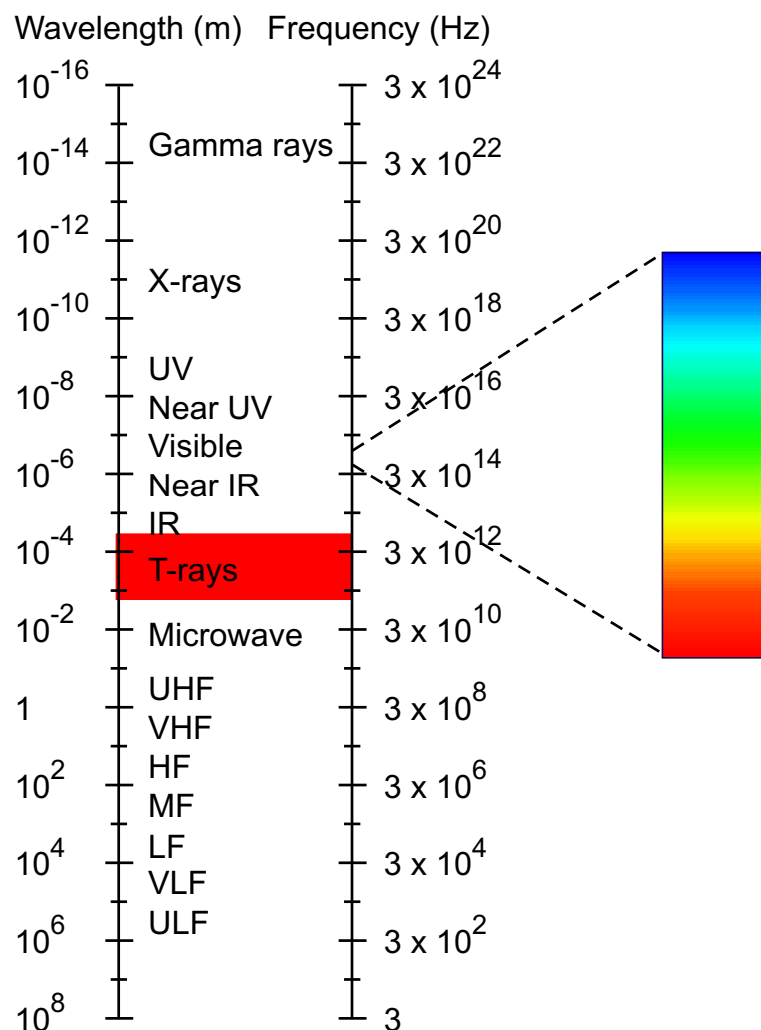


Figure 1.1. The electromagnetic spectrum. The THz (T-ray) frequency range lies in between microwave frequencies and the infrared portion of the optical spectrum. It is loosely defined by frequencies lying in between 100 GHz and 10 THz (wavelengths 3 mm to 30 μm).

or detector is tuned across the desired bandwidth and the sample's spectral response is measured directly. Both FTS and narrowband spectroscopy are also widely used in passive systems for monitoring thermal emission lines of molecules, particularly in astronomy applications.

Another, more recent technique is termed THz time-domain spectroscopy (THz-TDS). THz-TDS uses short pulses of broadband THz radiation, which are typically generated using ultrafast laser pulses. This technique grew from work in the 1980s at AT&T Bell Laboratories and the IBM T.J. Watson Research Center (Auston et al. 1984, Fattinger and Grischkowsky 1988). While the spectral resolution of THz-TDS is much coarser

than narrowband techniques (Xu et al. 2003), and its spectral range significantly less than that of FTS (Han et al. 2001), it has a number of advantages that have given rise to several important applications. The transmitted THz electric field is measured coherently, which provides both high sensitivity and time-resolved phase information. It is also amenable to implementation within an imaging system yielding rich spectroscopic images. A THz-TDS system is described in Fig. 1.2. Typical THz-TDS systems have a frequency bandwidth between 2 and 5 THz, a spectral resolution of 50 GHz, an acquisition time under one minute, and a dynamic range of 10^5 in electric field, or 10^{10} in power.

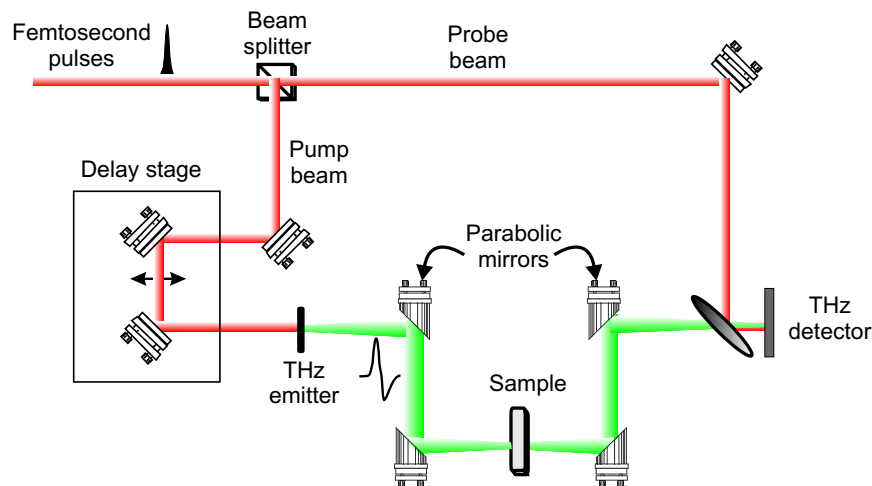


Figure 1.2. Illustration of a THz-TDS pump probe system. The ultrafast optical laser beam is split into pump and probe beams. The pump beam is incident on the THz emitter to generate THz pulses and the THz pulses are collimated and focused on the target using parabolic mirrors. After transmission through the target the THz pulse is collimated and re-focused on the THz detector. The optical probe beam is used to gate the detector and measure the instantaneous THz electric field. A delay stage is used to offset the pump and probe beams and allow the THz temporal profile to be iteratively sampled. Typically THz-TDS systems use lasers with a spectral wavelength in the 800 nm range, and are pulsed with pulse durations of the order of 100 fs.

1.3 Motivation

1.3.1 Three Dimensional THz Imaging Systems

Pulsed terahertz imaging was proposed by Hu and Nuss in 1995 (Hu and Nuss 1995). It is based upon the technique of terahertz time-domain spectroscopy (THz-TDS). Terahertz imaging has been demonstrated for imaging flames (Mittleman et al. 1999), scale-model aircraft (Cheville et al. 1997), leaf moisture content (Hadjiloucas et al. 1999), skin burn severity, tooth cavities (Ciesla et al. 2000) and skin tumours (Löffler et al. 2001).

Reflection mode THz tomography systems (Mittleman et al. 1997) are based on measuring the time-of-flight of reflected pulses. This technique is capable of resolving the 3D refractive index profile for objects consisting of well-separated layers of differing refractive index. This technique provides extremely sensitive range resolution of the order of $1\text{ }\mu\text{m}$, and is ideal for imaging targets such as the floppy disk shown in Fig. 1.3. It has been applied to a wide range of targets including the detection of oxidation underneath paint layers (Geltner et al. 2002) and biomedical targets including *in-vivo* dermal tissue (Cole et al. 2001b), and dental tissue (Crawley et al. 2002), where reflections arise from enamel, dentine and pulp boundaries (Ciesla et al. 2000). However, the current reconstruction algorithms are only valid given a number of assumptions that restrict its applicability (Mittleman et al. 1999). These algorithms neglect multiple reflections, absorption and dispersion in the object to be imaged. These restrictions have motivated research into more general tomographic imaging methodologies.

Other THz imaging algorithms, drawing inspiration from geophysical (Dorney et al. 2001b), radar (McClatchey et al. 2001) and optical diffraction (Ruffin et al. 2001) techniques, are capable of mapping the two and three dimensional distribution of scattering objects but have generally only been demonstrated for imaging the shape profile of the target object and both the internal structure and the optical properties of the sample are difficult to access. Kirchhoff migration has recently been demonstrated for determining the refractive index of internal layers (Dorney et al. 2002). However this technique is performed in the time domain and it is difficult to foresee its extension to dispersive targets and spectroscopic reconstruction. One focus, and important distinction, of this current work has been the development of techniques with the potential to extract the frequency dependent 3D properties of the target. This provides a rich

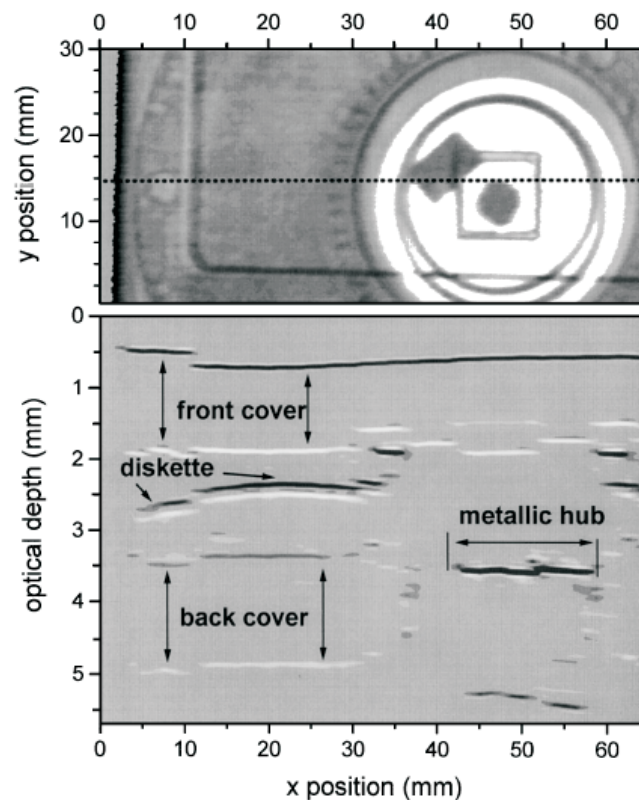


Figure 1.3. T-ray reflective tomography image of a floppy disk. A 3.5 inch floppy disk was imaged using a conventional reflective T-ray imaging system. The standard T-ray image is shown above. The image below shows a tomographic image of the same disk at a constant vertical (y) position, along the dashed line at $y = 15$ mm. The measured THz signals contained separate pulses arising from Fresnel reflections at each dielectric boundary. Algorithms were developed to extract the refractive index and thickness of each layer in the target based on the Fresnel reflection equations and the time of arrival of the reflected pulses. Dark stripes in the tomographic image indicate transitions from low to high refractive index media, while light stripes indicate transitions from high to low refractive index media. After (Mittleman et al. 1997).

four-dimensional data set that may be used to uniquely identify materials and may potentially have clinical diagnostic applications.

1.3.2 THz Inspection Systems

Terahertz wave (T-ray) sensing and imaging techniques have several advantages over other sensing and inspection imaging techniques. While microwave and X-ray imaging modalities provide density pictures, T-ray imaging also provides spectroscopic information within the THz frequency range. The unique rotational and vibrational responses of biological materials within the THz range provide information that is generally absent in optical, X-ray and NMR images. In addition, T-rays easily penetrate and image inside many dielectric materials, which are opaque to visible light and low contrast to X-rays, making T-rays a useful and complementary imaging source in this context.

T-rays offer an opportunity for transformational advances in security and manufacturing inspection. Numerous groups are working on demonstrating THz spectroscopy of explosives (Kemp 2003, Xu et al. 2003) and of bacterial spores (Brown et al. 2002, Globus et al. 2002, Woolard et al. 2001, Woolard et al. 1999, Walker et al. 1998).

1.4 Thesis Overview

*"You will see something new.
Two things. And I call them
Thing One and Thing Two."*

- Dr Seuss, The Cat in the Hat

This research seeks to advance the broad goal of *three dimensional THz inspection systems*. Perhaps as a result of the breadth and scope of this goal, this research encompasses several disparate disciplines; from quasi-optical imaging system design, to tomographic reconstruction algorithms, to the development of a signal processing classification framework. Nobel prize winner Linus Pauling is quoted as saying *"The best way to get a good idea is to get a lot of ideas."* (Rose and Nicholl 1998). In a similar vein Derek Abbott states that *"In any pioneering research program, the meandering path is seldom straight"* (Abbott 1995). These principles are reflected in this Thesis as numerous ideas are woven together and are unified in their potential for advancing 3D THz inspection systems. An overview of the Thesis structure is provided in Fig. 1.4.

In this Chapter the introduction, motivation and background are given, along with the current state of knowledge in the field and the key contributions presented in this

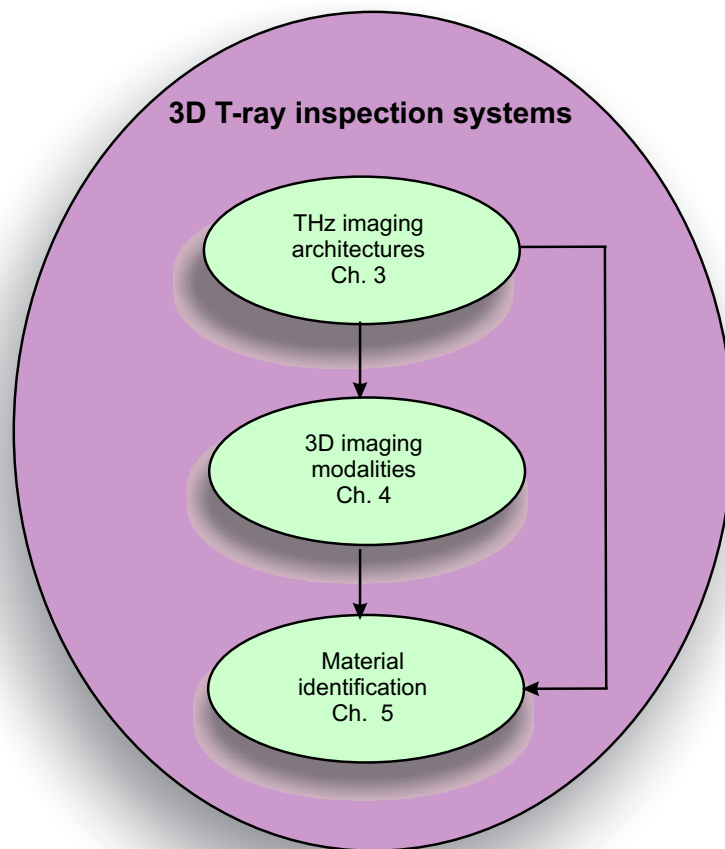


Figure 1.4. An overview of the Thesis structure. The major technical contribution of the Thesis may be grouped under four main headings. Work on THz imaging systems and pre-processing algorithms laid the groundwork for 3D imaging and material identification research. The material identification algorithms are general enough to be applied on both the 2D and 3D THz imaging data.

Thesis. The broader context of THz spectroscopy and imaging is illuminated in Ch. 2. It introduces THz generation and detection techniques whilst paying appropriate historical homage. To provide a sense of the potential of THz systems several recent applications are also discussed (Ferguson and Zhang 2002a).

Following this preamble, Ch. 3 describes the three distinct pulsed imaging architectures utilised in this research. The methods and specifications of each imaging architecture are provided in Ch. 3. Several innovative methods were developed to improve the signal-to-noise-ratio (SNR) and imaging speed. The techniques used for *synchronised dynamic subtraction* and EO sensor calibration are detailed.

Chapter 4 describes three novel tomographic imaging systems using pulsed THz radiation. T-ray holography (Ferguson et al. 2002d, Wang et al. 2003b) computed tomography (CT) (Ferguson et al. 2001b, Ferguson et al. 2002e, Ferguson et al. 2002b, Ferguson et al. 2002f) and diffraction tomography (DT) (Ferguson et al. 2002c, Ferguson et al. 2002c, Ferguson et al. 2003b) each drew inspiration from existing methods in other frequency bands. They required innovative hardware design, new reconstruction algorithms and in the case of T-ray CT, the derivation of a simplifying propagation model. T-ray CT and T-ray DT have the ability to image 3D targets and reconstruct the spectroscopic absorption coefficient and refractive index at each voxel. This provides the potential for automated detection of specific materials, which is the goal of the research described in Ch. 5.

Chapter 5 develops a classification framework for the identification of materials in pulsed THz images. Wavelet denoising and Wiener deconvolution are demonstrated as preprocessing techniques (Ferguson and Abbott 2001a, Ferguson and Abbott 2000, Ferguson and Abbott 2001b). They allow maximum information retention in the THz pulses whilst suppressing noise and unwanted characteristics. Two methods of feature extraction are proposed. The first uses a finite impulse response linear filter to model the THz response at each pixel and uses the filter coefficients as classification features (Ferguson et al. 2001c, Ferguson et al. 2002a). The second method uses the normalised, deconvolved amplitude and phase frequency coefficients as features. To reduce the dimensionality and improve the classification accuracy a genetic algorithm is developed to identify a subset of the available frequency components with optimal classification accuracy.

The second part of Ch. 5 applies the classification framework to three application-focused case studies. These case studies serve both to highlight the potential of THz inspection systems in different settings and to demonstrate the performance of the developed classification framework. The first case study considers biomaterial classification. Excised beef and chicken samples are imaged using the chirped probe pulse THz imaging system and are classified by species (Ferguson et al. 2001c, Ferguson et al. 2002a). The second case study considers the topical application of powder/anthrax detection inside envelopes (Ferguson et al. 2003c, Te et al. 2002, Wang et al. 2002a). The classification system is demonstrated in performing thickness independent classification of different powders. The final case study analyses the THz response of *in-vitro*

cultured normal and cancerous cells (Ferguson et al. 2003a). In all three case studies, high classification accuracies are demonstrated.

The major conclusions and future directions of this work are summarised in Ch. 6. Several appendices provide supporting information and technical details. Appendix A lists the major hardware components utilised in this work and provides their specifications. Appendix B, in turn, describes the software programs that were developed as part of this research and the third party software applications that were used to assist in data processing. The last three appendices reproduce important algorithms that support the results in this Thesis. Appendix C describes an algorithm used to extract the frequency dependent refractive index of a material from the THz-TDS measurements. Appendix D reproduces the original inversion formula for the Radon transform as derived by Radon (1917). Finally, Appendix E provides an example of the ‘Curse of Dimensionality’ after Trunk (1979).

1.5 Original Contributions

This Thesis makes a number of significant contributions to the body of THz science and technology.

Chapter 3 presents 2D THz imaging systems. Two-dimensional (2D) free-space electro-optic THz imaging systems are advanced by the development of a synchronised dynamic subtraction technique. This technique improves the SNR of THz imaging systems, when used in conjunction with low repetition rate regeneratively amplified lasers. An EO sensor calibration technique is also presented to further improve THz imaging results.

In collaboration with researchers at Rensselaer Polytechnic Institute several innovative 3D THz imaging systems are devised. A T-ray holography system is developed providing an order of magnitude improvement in acquisition speed over previous systems. A mathematical reconstruction algorithm is derived, based on the Windowed Fourier Transform (WFT), to allow T-ray holography to image 3D targets for the first time (Sec. 4.4).

The first published demonstration of diffraction tomography using pulsed THz radiation is performed. This system uses 2D free-space electro-optic THz imaging and linearisation of the Helmholtz equation to allow low contrast 3D targets to be imaged (Sec. 4.5).

Perhaps the most significant contribution of this Thesis is the invention of T-ray computed tomography. This technique required innovative optical design, the derivation of approximations to the Helmholtz equation and the development of reconstruction algorithms based on filtered backprojection. THz pre-processing algorithms are derived to allow existing backprojection techniques to be applied to reconstruct both the phase and amplitude response of the target using THz-TDS measurements.

The ability of T-ray computed tomography to reconstruct the frequency-dependent refractive index of a target is demonstrated and the resolution is shown to be an order of magnitude better than the conventional limit of standard tomography systems (Sec. 4.6). To improve the fidelity of T-ray CT reconstructions a number of innovative signal processing techniques are developed to estimate the phase of the THz signal: an interpolated cross-correlation technique is utilised in the time-domain, and extrapolated phase unwrapping is used in the frequency-domain.

On the material identification front a classification framework for THz spectroscopy is proposed. This framework encompasses preprocessing, feature extraction and classification techniques. Wavelet denoising of THz pulses is investigated experimentally and its performance quantified. Two feature extraction algorithms are developed. The first uses linear filter modeling to derive filter coefficients. The second uses the normalised, deconvolved Fourier coefficients as classification features. A genetic algorithm is developed to optimise the generalisation performance of a classifier by iteratively identifying near-optimal subsets of features (Ch. 5).

Finally, several experimental case studies are conducted to verify the performance of the classification framework. Thickness independent classification of powdered substances is investigated (Sec. 5.7), and the ability of THz imaging to identify cellular differences between normal human bone cells and human osteosarcoma cells is demonstrated (Sec. 5.8).

These contributions serve to advance the goal of the development of practical 3D THz inspection systems. They provide substantial improvements over the existing state-of-the-art and serve to extend THz applications to new and potentially ground-breaking realms.

Chapter 2

Historical Landscape

WE review the rich history of pulsed THz technology; from its early motivation at the start of the 20th century, through its burgeoning expansion in the 1990's, to its recent maturation and the proliferation of application-focused research. This Chapter sets the scene for this Thesis by providing motivation, background, and a sense of the culmination of a technology with astonishingly broad potential.

Recent years have seen a plethora of significant advances as higher power sources and more sensitive detectors open up a range of potential applications. Applications including semiconductor and high-temperature superconductor characterisation, tomographic imaging, label-free genetic analysis, cellular level imaging, and chemical and biological sensing have thrust THz research from relative obscurity into the limelight.

This review commences by focusing on the enabling technologies for the generation and detection of THz radiation, and then progresses to summarise a number of recently developed THz applications.

2.1 THz Sources

The lack of a high power, low-cost, portable, room-temperature THz source is the most significant limitation in modern THz systems. However there is a vast array of potential sources each with relative advantages, and advances in high-speed electronics, laser, and materials research continue to provide new candidates. Sources may be broadly classified as either incoherent thermal sources, broadband pulsed techniques, or narrowband, continuous wave (CW) methods.

2.1.1 Broadband THz Sources

The vast majority of broadband, pulsed THz sources are based on the excitation of different materials with ultrashort laser pulses. A number of different mechanisms have been exploited to generate THz radiation, including photocarrier acceleration in photoconducting antennas, second order non-linear effects in electro-optic crystals, plasma oscillations (Hashimshony et al. 2001), and electronic non-linear transmission lines (van-der-Weide et al. 2000). Presently, conversion efficiencies for all of these sources are very low (of the order of 10^{-6}), consequently average THz beam powers tend to be in the nW to μ W range – while the average power of the femtosecond optical source is in the region of 1 W.

Photoconduction and optical rectification are two of the most common approaches for generating broadband, pulsed THz beams. The photoconductive approach uses high-speed photoconductors as transient current sources for radiating antennas (Mourou et al. 1981, Fattinger and Grischkowsky 1988). Typical photoconductors include high resistivity GaAs, InP, and radiation damaged silicon wafers. Metallic electrodes are used to bias the photoconductive gap and form an antenna.

The physical mechanism for THz beam generation in photoconductive antennas begins with an ultrafast laser pulse (with a photon energy larger than the bandgap of the material, $\hbar\omega > E_g$), which creates electron-hole pairs in the photoconductor. The free carriers then accelerate in the static bias field to form a transient photocurrent, and

this fast time-varying current radiates electromagnetic waves. A large number of material parameters affect the intensity and the bandwidth of the resultant THz radiation. For efficient THz radiation, it is desirable to have rapid photocurrent rise and decay times. Thus semiconductors with small effective electron masses such as InAs and InP are attractive. The maximum drift velocity is also an important material parameter; it is generally limited by the intraband scattering rate or by intervalley scattering in direct semiconductors such as GaAs (Gornik and Kersting 2001, Leitenstorfer et al. 1999a, Leitenstorfer et al. 1999b). Since the radiating energy mainly comes from stored surface energy in the form of the static bias field, the THz radiation energy scales up with the bias and optical fluency (Darrow et al. 1991, Darrow et al. 1992). The breakdown field of the material is another important parameter as this determines the maximum bias that may be applied (Ferguson et al. 2001a). Photoconductive emitters are capable of relatively large average THz powers in excess of $40 \mu\text{W}$ (Zhao et al. 2002a) and bandwidths as high as 20 THz (Shen et al. 2003).

Optical rectification (OR) is an alternative mechanism for pulsed THz generation. It is based on the inverse process of the electro-optic effect (Bass et al. 1962). Again, femtosecond laser pulses are required, but in contrast to photoconducting elements where the optical beam functions as a trigger, the energy of the THz radiation in optical rectification comes directly from the laser pulse excitation. The conversion efficiency in optical rectification depends primarily on the material's nonlinear coefficient and the phase matching conditions. As illustrated in Fig. 2.1, OR is a second-order nonlinear effect, which relies on an electro-optic crystal with a non-zero second order $\chi^{(2)}$ coefficient. The ultrafast optical field is rectified in the crystal. The pump pulses induce an ultrafast transient polarisation, $P(t)$, which radiates at THz frequencies. The temporal THz pulse profile is given by the second time derivative of the polarisation transient $\partial^2 P / \partial t^2$ (Zhang et al. 1992a).

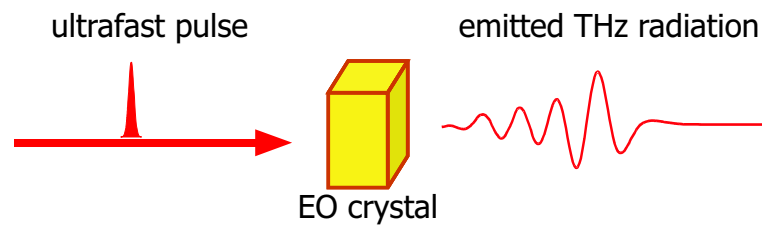


Figure 2.1. Illustration of optical rectification. The incident pump pulse induces a transient polarisation in a $\chi^{(2)}$ medium, this causes a transient pulse of broadband radiation at THz frequencies.

2.1 THz Sources

This technique was first demonstrated for generating far-infrared radiation using LiNbO₃ (Yang et al. 1971). Much research has focused on optimising THz generation through investigating the electro-optic properties of different materials including traditional semiconductors such as GaAs and ZnTe, organic crystals such as the ionic salt 4-dimethylamino-N-methyl-4-stilbazolium-tosylate (DAST) and many others (Zhang et al. 1992b, Rice et al. 1994, Zhang et al. 1992c, Han et al. 2000b, Ascazubi et al. 2004). Because optical rectification relies on relatively low efficiency coupling of the incident optical power to THz frequencies, it generally provides lower output powers than photoconductive antennas, but it has the advantage of providing very high bandwidths as high as 50 THz (Bonvalet et al. 1995). Phase matched optical rectification in GaSe allows ultra-broadband THz pulses to be generated with a tunable centre wavelength. Tuning up to a frequency of 41 THz is accomplished by tilting the crystal about the horizontal axis perpendicular to the pump beam to modify the phase matching conditions (Kaindl et al. 1999, Huber et al. 2000).

2.1.2 Narrowband THz Sources

Narrowband THz sources are crucial for high resolution spectroscopy applications. They also have broad potential applications in telecommunications, and are particularly attractive for extremely high bandwidth inter-satellite links. For these reasons there has been significant research interest in the development of narrowband sources in the last century (Wiltse 1984). A multitude of techniques are under development, including upconversion of electronic RF sources, downconversion of optical sources, lasers, and backward-wave tubes. Several comprehensive reviews of this field are available (Siegel 2002, Siegel 2004, Micken et al. 2000, Hadni 2003, Micken and Zhang 2003).

The most commonly employed technique for generating low power ($< 100 \mu\text{W}$) continuous wave (CW) THz radiation is through upconversion of lower frequency microwave oscillators such as voltage controlled oscillators and dielectric-resonator oscillators. Upconversion is typically achieved using a chain of planar GaAs Schottky diode multipliers (Chattopadhyay et al. 2004). Using these methods frequencies as high as 2.7 THz have been demonstrated (Maiwal et al. 2001). Research also continues to increase the frequency of Gunn and IMPATT diodes to the lower reaches of the terahertz region using alternate semiconducting structures and improved fabrication techniques (Ryzhii et al. 2002). Gas lasers are another common THz source. In these sources a CO₂ laser pumps a low pressure gas cavity, which lases at the gas molecule's

emission line frequencies. These sources are not continuously tunable and typically require large cavities and kW power supplies, however they can provide high output powers up to 30 mW. Methanol and HCN lasers are the most popular and they are in common use for spectroscopy and heterodyne receivers.

Extremely high power THz emissions have been demonstrated using synchrotrons and free electron lasers with energy recovering linear accelerators (Williams 2002, Carr et al. 2002, Chan et al. 2004). Free electron lasers use a beam of high-velocity bunches of electrons propagating in a vacuum through a strong, spatially varying magnetic field (Biedron et al. 2004). The magnetic field causes the electron bunches to oscillate and emit photons. Mirrors are used to confine the photons to the electron beam line, which forms the gain medium for the laser. Such systems impose prohibitive cost and size constraints and typically require a dedicated facility. However, they may operate CW or pulsed and provide average brightnesses more than six orders of magnitude higher than typical photoconductive antenna emitters. Free electron lasers have significant potential in applications where high power sources are essential or in the investigation of non-linear THz spectroscopy. A typical application is in near-field imaging of strongly-absorbing biological tissue (Schade et al. 2004). Bench top variations on the same theme, termed backward-wave tubes or carcinotrons, are also capable of providing mW output powers at THz frequencies and are commercially available (Kozlov and Volkov 1998).

A number of optical techniques have also been pursued for generating narrowband THz radiation. Original efforts began in the 1970s using nonlinear photomixing of two laser sources but struggled with low conversion efficiencies (Morris and Shen 1977). In this technique two CW lasers with slightly differing centre frequencies are combined in a material exhibiting a high second order optical non-linearity such as DAST. The two laser frequencies mutually interfere in the material to result in output oscillations at the sum and difference of the laser frequencies. These systems can be designed such that the difference term is in the THz range. Tunable CW THz radiation has been demonstrated by mixing two frequency-offset lasers in low temperature grown GaAs (Brown et al. 1995) and by mixing two frequency modes from a single multi-mode laser. Collinear mixing of dual wavelengths can offer broadly tunable output frequencies as wide as 2 to 20 THz (Taniuchi et al. 2004). Further techniques utilise optical parametric generators and oscillators where a Q-switched Nd:YAG laser pump beam generates a second idler beam in a nonlinear crystal and the pump and idler signal

beat together to emit THz radiation (Kawase et al. 1996, Shikata et al. 1999, Imai and Kawase 2001). An excellent review is provided in Kawase et al. (2003b). Optical techniques provide broadly tunable THz radiation, are relatively compact due to the availability of solid-state laser sources, and output powers in excess of 100 mW (pulsed) have been demonstrated (Kawase et al. 2001). Optical downconversion is a rich area for materials research as molecular beam epitaxy and other materials advances allow engineered materials with improved photomixing properties (Kadow et al. 2000).

Semiconductor lasers are a further technique with extreme promise for narrowband THz generation. The first such laser was demonstrated in lightly doped p-type germanium utilising hole population inversion induced by crossed electric and magnetic fields (Komiyama 1982). These lasers are tunable by adjusting the magnetic field or external stress. THz lasing in germanium has also been demonstrated by applying a strong uniaxial stress to the crystal to induce the hole population inversion (Gousev et al. 1999). Such lasers have a number of inherent limitations including low efficiency, low output power, and the need for cryogenic cooling to maintain lasing conditions. Recently, semiconductor deposition techniques have advanced to a level where the construction of multiple quantum well semiconductor structures for laser emission is feasible. Quantum cascade lasers were first demonstrated in 1994 based on a series of coupled quantum wells constructed using molecular beam epitaxy (Faist et al. 1994). A quantum cascade laser consists of coupled quantum wells (nanometre thick layers of GaAs sandwiched between potential barriers of AlGaAs). The quantum cascade consists of a repeating structure in which each repeat unit is made up of an injector and an active region. In the active region a population inversion exists and electrons transition to a lower energy level emitting photons at a specific wavelength. The electrons then tunnel between quantum wells and the injector region couples them to the higher energy level in the active region of the subsequent repeat unit.

Quantum cascade lasers have been demonstrated within the infrared spectrum but until very recently a number of significant problems had prevented THz quantum cascade lasers from being realised. The principle problems are caused by the long wavelength of THz radiation. This results in a large optical mode that causes poor coupling between the small gain medium and the optical field and high optical losses due to free electrons in the material (these losses scale as the square of the wavelength). Köhler et al. (2002) addressed these and other problems in their innovative design of a THz quantum cascade laser operating at 4.4 THz. The laser consisted of 104 repetitions of

the repeat unit (shown in Fig. 2.2) and a total of over 700 quantum wells. This original system demonstrated pulsed operation at a temperature of 10 K, however recent progress has resulted in continuous wave lasing above liquid nitrogen temperatures at 93 K (Kumar et al. 2004), and pulsed mode operation at up to 137 K (Williams et al. 2003). Work continues to further extend the lasing wavelength beyond $141\ \mu\text{m}$ (2.1 THz) (Williams et al. 2004).

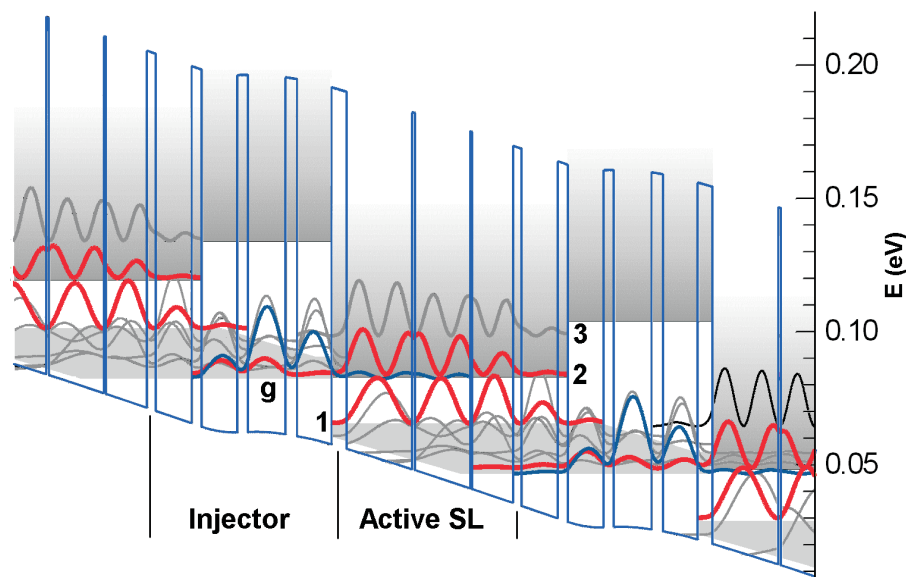


Figure 2.2. Conduction band structure of a THz quantum cascade laser. The waveguide core consists of alternating layers of injector and superlattice (SL) active regions. The moduli squared of the wavefunctions are shown, and the miniband regions are shown as shaded areas. Electrons are injected through a 4.3 nm AlGaAs injection barrier into the level 2 energy state of the active region from the injector ground state labeled *g*. The active transition from level 2 to level 1 results in the emission of 4.4 THz photons. The electrons then escape to the subsequent injector band. Here, 104 repeats of the basic 7 well structure are used in the laser. Each quantum well consists of a thin layer (10 - 20 nm) of GaAs between two potential barriers of AlGaAs (0.6-4.3 nm thick). The *x*-axis of the figure is proportional to the layer thicknesses. The layer thicknesses and the applied electric field are tuned provide the required tunneling characteristics. After (Köhler et al. 2002).

2.2 THz Detectors

The detection of THz frequency signals is a complementary area of active research. The low output power of THz sources coupled with relatively high levels of thermal background radiation in this spectral range necessitates highly sensitive detection methods. For broadband detection direct detectors based on thermal absorption are commonly used. Most of these require cooling to reduce the thermal background. The most common systems are helium-cooled silicon, germanium and InSb bolometers. Pyroelectric IR detectors may also be used at THz frequencies. Superconductor research has yielded extremely sensitive bolometers based on the change of state of a superconductor such as niobium. Interferometric techniques may be used to extract spectral information using direct detectors. A single photon detector for THz photons has been demonstrated (Komiyama et al. 2000). This detector offers unparalleled sensitivity using a single electron transistor consisting of a quantum dot in a high magnetic field. Although detection speeds are currently limited to 1 ms, high speed designs are proposed and this has the potential to revolutionise the field of THz detection.

In applications requiring very high sensor spectral resolution heterodyne sensors are preferred. In these systems a local oscillator (LO) source at the THz frequency of interest is mixed with the received signal. The downshifted signal is then amplified and measured. At room temperature semiconductor structures may be used. A planar Schottky diode mixer has been operated successfully at 2.5 THz for space sensing applications (Gaidis et al. 2000). For higher sensitivity, cryogenic cooling is used for heterodyne superconductor detectors. Several superconductor structures can be used and have been since the 1980's. The most widely used is the superconductor-insulator-superconductor tunnel junction mixer (Dolan et al. 1979). High temperature superconductors such as YBCO are under investigation for their potentially higher bandwidth operation. A number of general reviews of narrowband THz receivers are available (Carlstrom and Zmuidzinas 1996). Alternative narrowband detectors such as electronic resonant detectors, based on the fundamental frequency of plasma waves in field effect transistors have been demonstrated up to 600 GHz (Knap et al. 2002).

For pulsed THz detection in THz-TDS systems, coherent detectors are required. The two most common methods are based on photoconductive sampling and free-space electro-optic sampling (FSEOS), both of which rely on ultrafast laser sources. Fundamentally, the electro-optic effect is a coupling between a low frequency electric field

(THz pulse) and a laser beam (optical pulse) in the sensor crystal. Simple tensor analysis indicates that using a $\langle 110 \rangle$ oriented zincblende crystal as a sensor provides the highest sensitivity. The THz electric field modulates the birefringence of the sensor crystal; this in turn modulates the polarisation ellipticity of the optical probe beam passing through the crystal. The ellipticity modulation of the optical beam can then be polarisation analysed to provide information on both the amplitude and phase of the applied electric field (Valdmanis et al. 1983, Wu and Zhang 1995). A typical schematic for FSEOS is shown in Fig. 2.3.

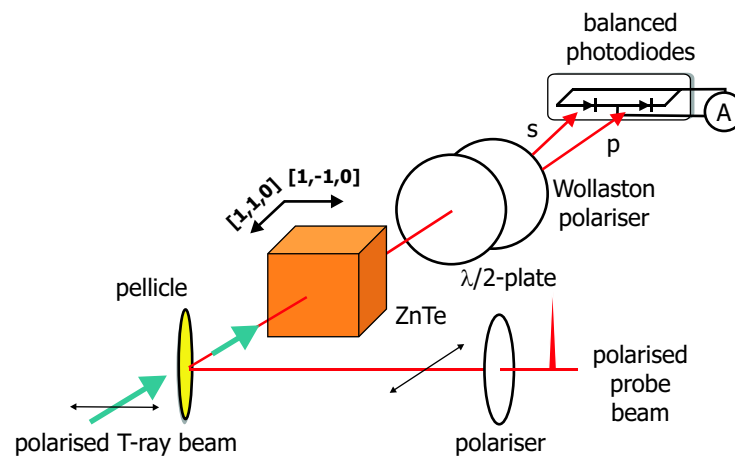


Figure 2.3. Illustration of free space electro-optic sampling. The polarised T-ray electric field induces a birefringence in the detector, depending on the $\chi^{(2)}$ coefficient of the specific crystallographic orientation of the crystal (Chen et al. 2001). A pellicle beam-splitter directs the THz and probe beam collinearly through the EO detector. The polarisation of the probe beam is rotated by the birefringent crystal, and this is converted to an intensity modulation using an analyser. The analyser shown here is a Wollaston beam splitter, it directs the two polarisations of the probe beam to balanced photodiodes. The resultant beam polarised normal to the plane of incidence is referred to as the *s*-polarisation, while the beam polarised parallel to the plane of incidence has *p*-polarisation. A half-wave plate is rotated to balance the difference current to zero for zero THz field, accounting for residue birefringence in the EO crystal. After (Lu et al. 1997).

The use of an extremely short laser pulse (< 15 fs) and a thin sensor crystal ($< 30 \mu\text{m}$) allow electro-optic detection of signals into the mid-IR range. Figure 2.4a shows a mid-IR pulsed THz waveform. The Fourier transform of the THz pulse is shown in Fig. 2.4b; note that the highest frequency response reaches over 30 THz (Han et al. 2001). The resonant absorption at 5.3 THz is due to the phonon modes of the ZnTe

2.2 THz Detectors

crystals. Extremely high detection bandwidths, in excess of 100 THz, have been demonstrated using thin sensors (Brodschelm et al. 2000). ZnTe is a popular crystal for EO detection as a result of its high EO coefficient and good mechanical properties. Several other crystals have also shown promise, including LiTaO₃, DAST (Wu and Zhang 1995) and GaSe (Liu et al. 2004).

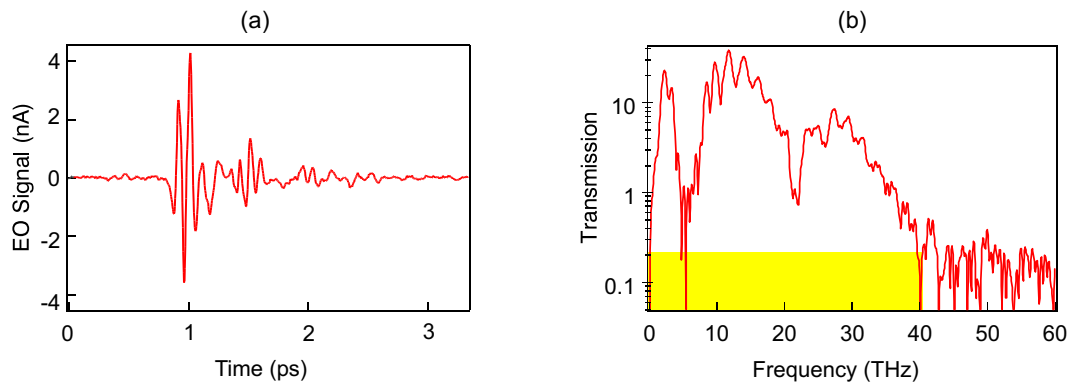


Figure 2.4. A broadband THz pulse. (a) Temporal waveform of a THz pulse generated using optical rectification in a 27 μm thick ZnTe emitter and measured using free space electro-optic sampling in a 30 μm thick ZnTe sensor. (b) Frequency spectrum of the THz field. The frequency spectrum extends into the infrared. The absorption resonance at 5.3 THz is due to phonon modes in the ZnTe crystals. The shaded region indicates the effective bandwidth of the pulse, which extends to 40 THz. After (Han et al. 2001).

Photoconductive antennas are also widely used for pulsed THz detection. An identical structure to the photoconductive antenna emitter may be used. Rather than applying a bias voltage to the electrodes of the antenna, a current amplifier and ammeter are used to measure the transient current generated by an optical pulse and biased by the instantaneous THz field. THz-TDS systems based on photoconductive emitters and receivers have been demonstrated with flat spectral responses between 0.3 and 7.5 THz (Shen et al. 2004). Ultrahigh bandwidth detection has also been demonstrated using photoconductive antennas detectors with detectable frequencies in excess of 60 THz (Kono et al. 2001, Kono et al. 2002).

A Michaelson interferometer-based detection scheme may be used to improve the sensitivity of THz detectors. In these systems the THz beam is split into two paths, one of which is focused on the target. The two beams are coherently combined to form an interference pattern on the detector (Krishnamurthy et al. 2001). This technique has been demonstrated for sensitive imaging of thin films (Johnson et al. 2001).

2.3 THz Applications

“... physicists, like theologians, are wont to deny that any system is in principle beyond the scope of their subject.”

Paul Davies (Davies and Brown 1988)

One of the primary motivations for the development of THz sources and spectroscopy systems is the potential to extract material characteristics that are unavailable using other frequency bands. Astronomy and space research has been one of the strongest drivers for THz research due to the vast amount of information available concerning the presence of abundant molecules such as oxygen, water and carbon monoxide in stellar dust clouds, comets and planets (Holland et al. 1998). It is estimated that approximately 98% of the photons in the universe lie in the submillimetre and far-IR frequency range (Siegel 2002). In recent years THz spectroscopy systems have been applied to a huge variety of materials both to aid the basic understanding of the material properties and to demonstrate potential applications in sensing and diagnostics. This section briefly reviews several crucial applications.

2.3.1 Material Characterisation

One of the major applications of THz spectroscopy systems is in material characterisation, particularly of lightweight molecules and semiconductors. THz spectroscopy has been used to determine the carrier concentration and mobility of doped semiconductors such as GaAs and silicon wafers (van Exter et al. 1989, van Exter and Grischkowsky 1990b, Grischkowsky et al. 1990). The Drude model may then be used to link the frequency dependent dielectric response to the material free carrier dynamic properties including the plasma angular frequency and the damping rate (van Exter and Grischkowsky 1990a). An important focus is on the measurement of the dielectric constant of thin films (Chen et al. 1999). THz spectroscopy is capable of highly sensitive gas detection down to part-per-million sensing of methyl chloride (Harmon and Cheville 2004). It may even be used for ‘watching paint dry’ (Yasui et al. 2003).

High temperature superconductor characterisation is another important application of THz spectroscopy (Frenkel et al. 1996). A large number of superconducting thin films have been analysed to determine material parameters including the magnetic penetration depth and the superconducting energy gap (Demsar et al. 2004). THz-TDS has

2.3 THz Applications

been used to study the newly discovered superconducting material MgB_2 . This material exhibits an extremely high transition temperature of 39 K and is currently not well understood. THz-TDS was used to determine the superconducting gap energy threshold of approximately 5 meV. This corresponds to only half the value predicted by current theory and points to the existence of complex material interactions (Kaindl et al. 2002). THz techniques have also been demonstrated for visualisation of the supercurrent distribution in high transition temperature (T_c) superconductors (Hangyo et al. 1999).

Optical pump-THz probe experiments may be performed to reveal additional information about materials. In these experiments the material is excited using an ultrafast optical pulse and a THz pulse is used to probe the dynamic far-infrared optical properties of the excited material. Huber et al. (2001) used an optical-pump THz-probe system to identify the time evolution of charge-charge interactions in an electron-hole plasma excited in GaAs using ultrafast optical pulses. This work added experimental evidence to quantum-kinetic theoretical predictions regarding charge build-up or ‘dressed quasi-particles’.

2.3.2 THz Imaging

Pulsed THz wave imaging, or ‘T-ray imaging’, was first demonstrated by Hu and Nuss (1995), and since then has been used for imaging a wide variety of targets including semiconductors (Mittleman et al. 1996), organic solvents (Mickan et al. 2002b), cancerous tissue (Löffler et al. 2001) and flames (Cheville and Grischkowsky 1995a). The attraction of THz imaging is largely due to the availability of phase-sensitive spectroscopic images, which holds the potential for material identification or *functional* imaging.

THz systems are ideal for imaging dry dielectric substances including paper, plastics and ceramics. These materials are relatively non-absorbing in this frequency range, yet different materials may be easily discriminated on the basis of their refractive index, which is extracted from the THz phase information. Many such materials are opaque at optical frequencies and provide very low contrast for X-rays. THz imaging systems may therefore find important niche applications in security screening and manufacturing quality control.

A notable application focus has been on imaging of insulating foam such as that used to insulate space shuttle fuel tanks. This application has received much attention due to the space shuttle Columbia disaster on February 1, 2003. A piece of foam was dislodged during launch and damaged the shuttle wing. This damage is believed to have caused the destruction of the shuttle on re-entry. THz imaging holds promise for imaging disbonds (voids) underneath the foam to identify defects that could cause future disasters. Principle advantages of THz imaging are the high resolution available and the fact that the foam is relatively transparent at THz frequencies (Zandonella 2003). Figure 2.5 shows a large foam block mounted in a THz imaging system.

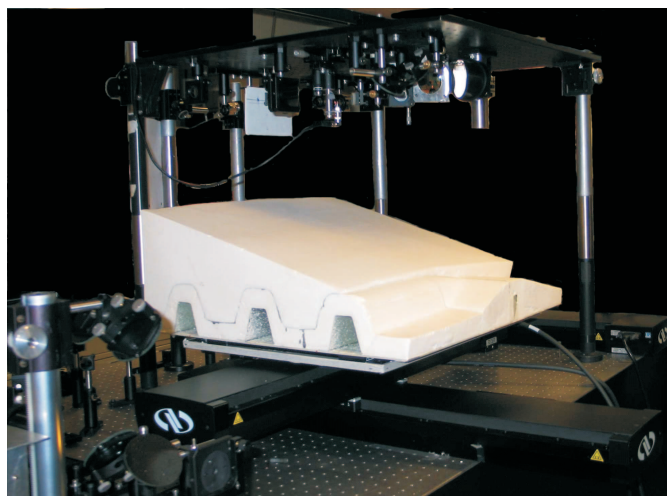


Figure 2.5. Foam used to insulate space shuttle fuel tanks. The insulating foam may be imaged using THz imaging to identify disbonds (voids underneath the foam) that could lead to the foam dislodging during launch. Image courtesy of X.-C. Zhang.

There is also increasing interest in using THz imaging to study cellular structure. A fundamental limitation in this context is the resolution of current systems. The Rayleigh criterion limits the far field resolution of an imaging system to the order of the wavelength (0.3 mm at 1 THz). For this reason researchers are relying on imaging in the near field to achieve improved spatial resolution. Using near field aperture-based techniques, similar to those used in near field optical microscopy, resolutions of 7 μm have been demonstrated using radiation with a centre wavelength of 600 μm (Mitrofanov et al. 2001b). In these methods, a subwavelength sized aperture is placed at the focal point of the THz beam and the sample is placed in the near-field of the aperture (Hunsche et al. 1998). Non-aperture based near-field techniques utilising an oscillating metal tip to modulate the detected field have proven capable of extending THz imaging resolutions even further, down to 150 nm (Chen et al. 2003).

2.3 THz Applications

An alternative method to improve the resolution is to use higher frequency THz pulses (Han and Zhang 1998a). Figure 2.6 shows a THz image of a membrane of onion cells. The resolution of approximately $50\text{ }\mu\text{m}$ is achieved by using very broadband THz pulses extending into the mid-infrared. The contrast in the image is attributed primarily to differences in the water content of the cells and the intercellular regions (Han et al. 2000b).

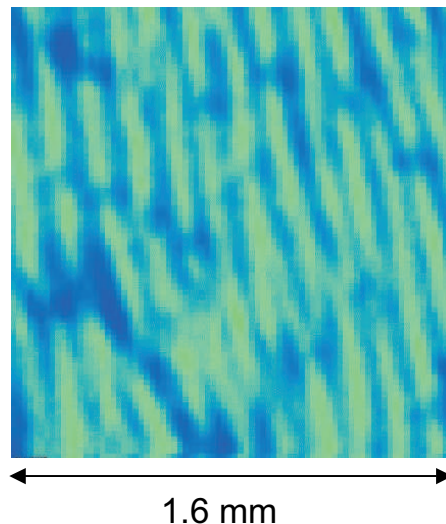


Figure 2.6. THz image of an onion cell membrane. A THz imaging system based on optical rectification and free space electro-optic sampling in $30\text{ }\mu\text{m}$ thick ZnTe crystals was used with a bandwidth up to 40 THz. This allowed a spatial resolution of less than $50\text{ }\mu\text{m}$ to be achieved. The cellular structure of the tissue membrane is clearly visible. After (Han et al. 2000b).

2.3.3 Biomaterial THz Applications

THz systems have broad applicability in a biomedical context (Siegel 2004). Active fields of research range from cancer detection (Woodward et al. 2001) to drug discovery (Taday et al. 2003) to genetic analysis (Nagel et al. 2002). Biomedical applications of THz spectroscopy are facilitated by the fact that the collective vibrational modes of many proteins and DNA molecules are predicted to occur in the THz range (Markelz et al. 2000). THz spectroscopy has also been heralded for its potential ability to infer information on a biomolecule's conformational state. The complex refractive index of pressed pellets consisting of DNA and other biomolecules have been determined and found to show absorption consistent with a large density of low frequency IR active

modes (Markelz et al. 2000, Walther et al. 2000, Fischer et al. 2002). Globus et al. (2003) demonstrated the ability of normal mode analysis to model the far-infrared response of DNA and RNA molecules and showed experimental verification of these results.

DNA analysers are used to identify polynucleotide base sequences for a variety of genetic applications. Gene chips are an increasingly popular technique where DNA fragments are typically bound to fluorescently labeled polynucleotides with known base sequences (Duggan et al. 1999). Fluorescent labeling can affect diagnostic accuracy and increases the cost and preparation time of gene-chips. As a result a large number of 'label-free' methods are being researched. THz imaging appears to hold promise in this context. THz spectroscopy has shown the capability to differentiate between single and double stranded DNA due to associated changes in refractive index (Brucherseifer et al. 2000). The same group has also demonstrated a THz sensing system capable of detecting DNA mutations of a single base pair with femtomol sensitivity (Nagel et al. 2002).

A further biomedical application of THz systems is the T-ray biosensor (Mickan et al. 2002d, Mickan et al. 2002e). A simple biosensor has been demonstrated for detecting the glycoprotein avidin after binding with vitamin H (biotin). A film of avidin is deposited on a solid substrate as shown in Fig. 2.7(a) and half of the biosensor slide is exposed to the environment or solution of interest. Avidin has a very strong affinity for biotin and binds to any biotin-containing molecules. The modified far infrared optical properties of the bound avidin film can then be detected using the technique of differential THz-TDS (Mickan et al. 2002c, Mickan et al. 2002a). The slide is mounted on a galvanometric shaker and the THz beam is alternately focused through the biotin and the control portion of the slide as illustrated in Fig. 2.7(b). Comparing the signal measured using a slide treated with 0.3 ng/cm^2 biotin solution with a plain avidin slide revealed an easily detectable signal shown in Fig. 2.7(c). This detectable limit is significantly enhanced by chemically binding the avidin molecules to agarose beads to provide an increased refractive index contrast (Menikh et al. 2002). Such techniques may find broad application in trace gas sensing and proteomics.

2.4 Outlook

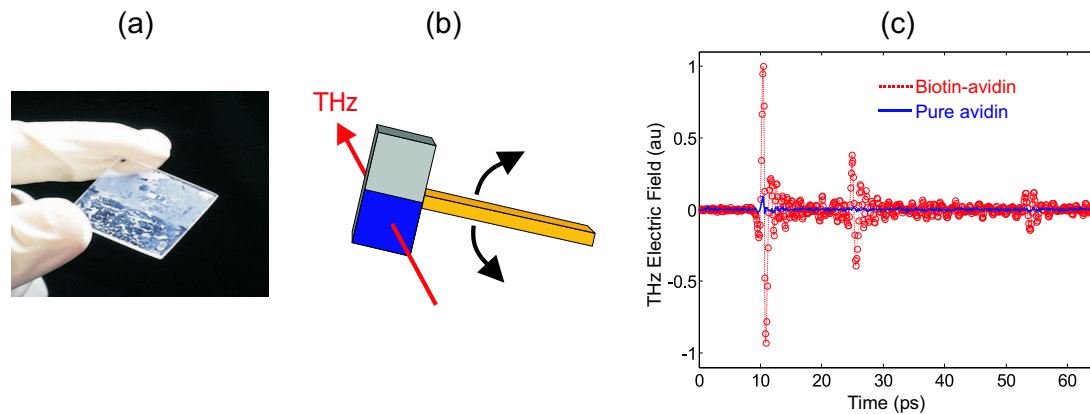


Figure 2.7. A biotin-avidin T-ray biosensor. (a) A photo of the test slide, which was coated with an avidin thin film, and half the slide was exposed to a biotin solution. (b) Illustration of the measurement procedure where the slide is mounted on a galvanometric shaker and translated back and forth in the THz beam to allow the differential signal to be measured. (c) The THz pulse measured after transmission through the avidin-biotin sensor with (dashed line) and without (solid line) exposure to 0.3 ng/cm^2 of biotin molecules chemically bound to agarose beads in solution. After (Mickan et al. 2002a).

2.4 Outlook

THz spectroscopy systems have undergone dramatic changes over the past decade. Improved source and detector performance continue to enable new application areas and facilitate the transition of THz systems from the laboratory to commercial industry. Biomedical imaging and genetic diagnostics are two of the most obvious potential applications of this technology, but equally promising is the ability to investigate material characteristics, probe distant galaxies, and study quantum interactions. THz radiation will continue to find revolutionary new uses, such as in the manipulation of bound atoms, which holds potential for future quantum computers (Cole et al. 2001a). Higher power THz sources will give rise to non-linear THz spectroscopy, with the potential to extract additional material characteristics. The THz band has a rich science replete with numerous promising applications. There are a number of key research areas that promise significant continuing advances in THz technology. Central among these are current efforts towards higher power THz sources, higher sensitivity detectors, and improved understanding of the interaction between THz radiation and materials such as quantum structures and biomaterials. Equally important are engineering considerations such as the development of high speed imaging systems and algorithms for accurately processing THz data such as form the focus of this Thesis.

Chapter 3

THz Imaging

PULSED THz imaging systems are a recent addition to the wide array of available imaging modalities. The unique properties of THz radiation allow THz imaging to fill niches that are unreachable using other techniques. This Chapter reviews the range of available THz imaging techniques and details the hardware systems used in this research.

The primary measures of the quality of an imaging system are its resolution, acquisition speed and signal to noise ratio. The performance of THz imaging systems are quantified under these criteria. Several innovative methods were developed to improve on existing THz imaging hardware systems to facilitate research into three dimensional imaging and material identification.

3.1 Introduction

“Suicide bombers, plastic explosives strapped to their bodies, approach the turnstiles at a packed football stadium. The security guards don’t have time to search every spectator, and even if a metal detector were installed, it would miss the terrorists’ deadly cargo. But a novel device that can see through the bombers’ clothing succeeds where other systems fail. Security personnel are alerted, and surround the attackers before they can strike.”

Zandonella (2003)

Imaging systems are an indispensable part of modern day life. They are used to record our television shows and our family memories, to protect our homes, to scan our luggage and probe our bodies for disease. A multitude of different imaging systems exist and each has found its application as a result of its unique properties. THz imaging systems, despite representing a young and immature technology, have a number of intrinsic advantages propelling them forward.

This Chapter begins by introducing THz imaging systems and discussing several of the prominent challenges in this field. It then lays a foundation for future chapters by detailing the three imaging architectures utilised in this research on 3D imaging (Ch. 4) and material identification algorithms (Ch. 5). Each imaging technique has advantages and disadvantages, and these are discussed. Several methods were implemented to improve the SNR and speed of THz imaging and these are also presented.

3.1.1 Passive THz Imaging

Radiation is emitted by all objects in the universe with a temperature above 0 Kelvin. This radiation is emitted as a result of the vibration of molecules and is broadband, covering a broad range of the electromagnetic spectrum. The distribution of the radiation with frequency is temperature dependent and is governed by Planck’s Law. It describes the radiation intensity emitted by a blackbody (perfect radiator) at a temperature T as a function of wavelength, λ . Planck’s Law is given by

$$M_{\lambda} = \frac{2\pi hc^2}{\lambda^5} \left(\frac{1}{\exp \left[\frac{hc}{\lambda kT} \right] - 1} \right), \quad (3.1)$$

where M_λ is the spectral radiant exitance of a blackbody, $h = 6.626 \times 10^{-34}$ Js is Planck's constant and $k = 1.3805 \times 10^{-23}$ J/K is the Boltzmann constant. In general, the higher the temperature of an object, the more radiation it will emit, and the higher the frequency of the peak of the radiation. Cool interstellar dust emits radiation with a peak wavelength in the THz range, while objects at room temperature (around 300 K) emit mostly in the infrared region. Figures 3.1 and 3.2 show the radiation distributions at different temperatures.

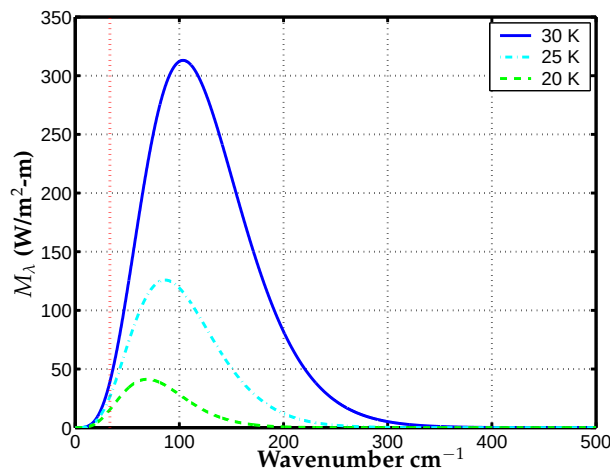


Figure 3.1. Spectrum of blackbody radiation at low temperatures. At low temperature the peak of the intensity distribution lies in the THz range. The distributions at 15 K, 20 K and 25 K are shown. The dashed vertical line indicates the wavenumber at 1 THz. The wavenumber is a unit commonly employed by spectroscopists and is defined as the inverse of the wavelength ($1/\lambda$). The frequency range 0.1 to 10 THz corresponds to wavenumbers 3.3 to 333.3 cm^{-1} .

Thus the universe is bathed in a glow of THz radiation, much of which is radiated by cool (30 K) stellar dust. The oldest form of THz imaging is passive submillimetre sensing, which has been used for many decades for space imaging applications. In these systems a heterodyne detector (most often aboard a satellite) is used to sense the amount of THz radiation emitted by distant galaxies. By tuning the frequency of the detector a spectrum can be obtained, and this spectrum contains vital information regarding the presence of certain molecules in that distant galaxy. For instance, water molecules have strong characteristic absorption resonances at 0.557 THz, 0.752 THz, 1.097 THz, 1.113 THz, 1.163 THz and 1.207 THz (Pickett et al. 2003, Pickett et al. 1998, Poynter and Pickett 1985). By comparing the amplitude of the received THz power at these frequencies relative to the background radiation, astronomers can determine whether water is likely to exist on distant planets. This is a vital tool in the search for

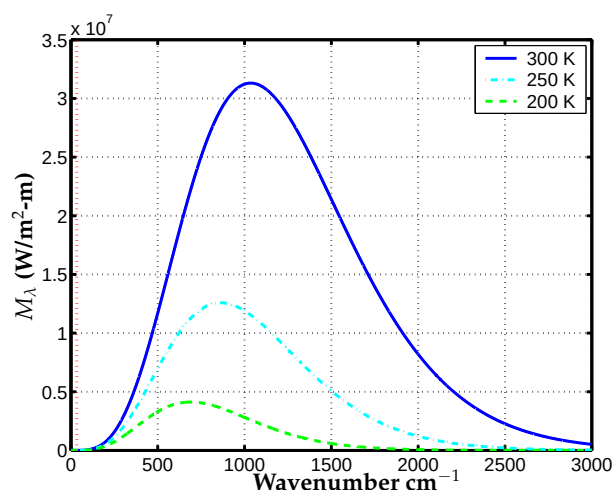


Figure 3.2. Spectrum of blackbody radiation at ambient temperatures. At higher temperatures the peak of the intensity distribution lies in the IR range. The distributions at 200 K, 250 K and 300 K are shown. The vertical line indicates the wavenumber at 1 THz.

extraterrestrial life. Other molecules that can be easily identified using this technique include oxygen, carbon monoxide and nitrogen (Siegel 2002).

Similarly, passive THz imaging principles have been employed in terrestrial applications. This type of imaging system is aided by the fact that a wide variety of common materials have very low absorption coefficients at THz frequencies and thus appear transparent to THz imaging systems. Materials such as plastics, cloth, paper, cardboard, and even many building materials are transparent at THz frequencies yet totally opaque in the optical spectrum. Figure 3.3 shows a pulse of broadband THz radiation after transmission through a wide variety of clothing. The THz pulse is detected after transmission through most clothing types. Bjarnason et al. (2004) have characterised the far-infrared spectral response of a number of types of fabric using FTIR spectroscopy and shown that nylon and rayon are particularly transparent.

This led groups such as the European Space Agency (ESA) (Mann et al. 2003) to invest heavily in the development of a passive CCD camera operating at THz frequencies. This project focused on combining micro-machined terahertz antennas with a silicon photonic band gap backing plane to form an imaging array. A prototype of this camera is demonstrated in Fig. 3.4, where a man is imaged with an object under his shirt. The object is clearly identified in the THz image. The camera obtains THz images at frequencies of 0.25 THz and 0.3 THz.

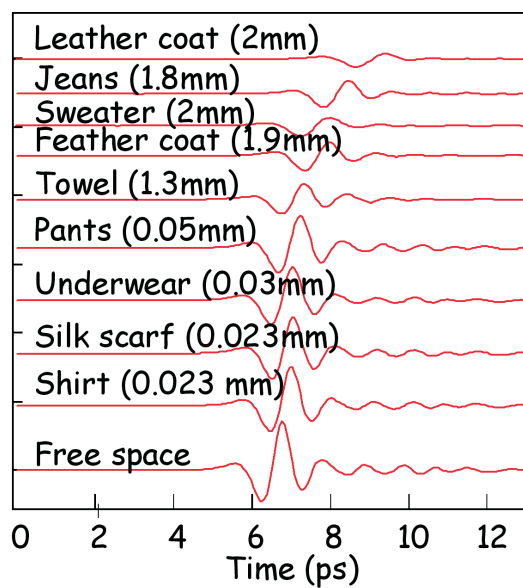


Figure 3.3. THz pulse measured after transmission through various types of clothing. Most types of clothing, and many other materials transmit THz radiation with minimal absorption. This provides the potential for many inspection imaging applications. After (Zhang 2003).

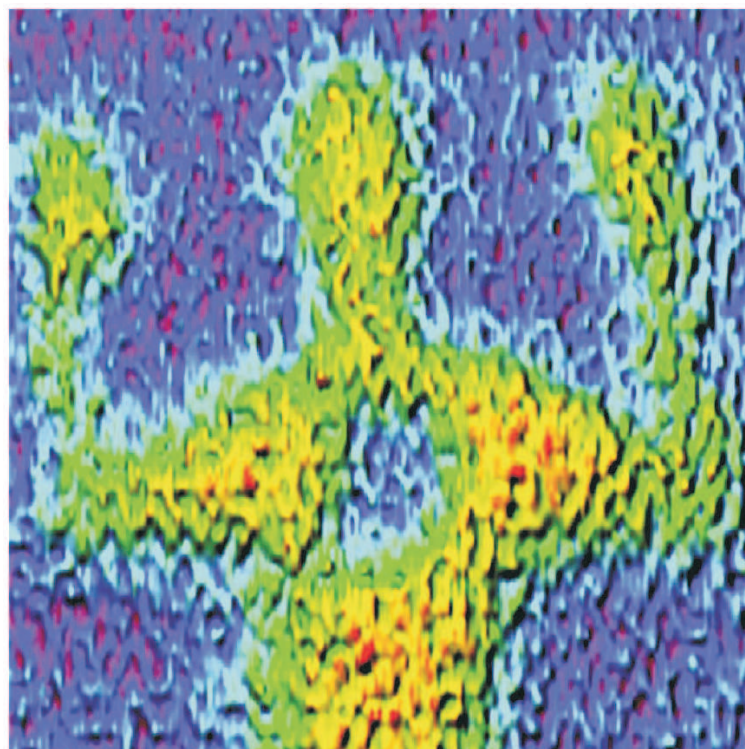


Figure 3.4. Passive THz image of a man. The person's outline is clearly identified as is an object under the person's clothing near his chest (shown as blue). The passive THz imager collects THz radiation at 0.25 THz and 0.3 THz. After (Zandonella 2003).

3.1.2 Active THz Imaging

While the fact that all objects emit THz radiation does in fact enable passive imaging techniques, it is also a severe source of noise. For this reason, passive THz imaging methods have had most success in space, where the detector can be mounted on a satellite, away from the strong thermal background that exists on Earth and directed solely at the target of interest.

Active imaging refers to the technique of illuminating the target with a source of radiation, and then measuring the reflected or transmitted radiation. A well known example of active imaging is radar. A typical radar system emits pulses of radiation at a particular frequency, and often with a particular modulation. The receiver detects the reflected radiation and looks for the same frequency and modulation; this allows the radar to detect a weak signal in the presence of strong background noise. Based on the time delay of the received pulse and its direction, the location of the target can be accurately determined (Stimson 1998).

Active imaging systems can use a pulsed or continuous wave (CW) illumination. Early THz imaging systems used CW gas THz lasers to illuminate the target and thermal detectors (Malykh et al. 1975, Hartwick et al. 1976) or pyroelectric cameras (Lash and Yundev 1984). Generally pulsed systems are preferred as they use a much lower average illumination power. Thermal background noise is a common problem in active imaging systems. Passive radiation emitted by the target or the surroundings is generally indistinguishable from the active illumination return, resulting in noise in the image. It is desirable, therefore, that the illumination power is significantly higher than the thermal background noise power. For pulsed systems the illumination power is compressed into a short pulse width (typical pulsed THz systems have a pulse width of a few picoseconds 10^{-12} s). This results in a very high *peak* illumination power. Using coherent detection methods to detect the instantaneous THz power, rather than the time averaged value, allows much lower average power sources to be used while providing the same signal to noise ratio (SNR). For example, van Exter and Grischkowsky (1990b) calculated the *average* noise current generated by the thermal background to be 1.4×10^{-15} A compared to the *peak* current generated by the THz pulses in their THz-TDS system of 1.8×10^{-2} A.

3.2 THz Imaging Horizons and Hurdles

Terahertz (THz) science has tremendous potential for applications in fields as diverse as medical diagnosis, health monitoring, environmental control and chemical and biological identification. THz band research has been widely viewed as one of the most promising research areas in the 21st century for transformational advances in imaging, as well as in other interdisciplinary fields (Zhang 2002). However, terahertz wave (T-ray) imaging is still in its infancy. This section discusses the uniqueness and limitations of T-ray imaging, identifies the major challenges impeding T-ray imaging and proposes solutions and opportunities in this field.

3.2.1 Horizons and Goals

Several properties of THz wave radiation triggered research to develop this frequency band for imaging applications. T-rays have low photon energies (for example, 4 meV @ 1 THz) and therefore do not subject biological tissue to ionising radiation (Smye et al. 2001, Walker et al. 2002). In comparison, a typical X-ray photon has an energy in the keV range, which is 1 million times higher than a T-ray photon, causing ionisation and other potentially harmful effects.

While microwave and X-ray imaging modalities produce density pictures, T-ray imaging has the additional capability of providing spectroscopic information within the terahertz (THz) frequency range. The unique rotational, vibrational, and translational responses of materials within the THz range provide information that is generally absent in optical, X-ray and NMR images². In principle, these transitions are specific to the molecule and therefore enable THz wave fingerprinting. For large molecules THz frequency resonances correspond to conformational (tertiary structure) changes and this provides information that is closely related to biological functions of the molecules in tissues and cells and is difficult to access with other techniques. Coherent THz wave signals are detected in the time-domain by mapping the transient of the electric field in amplitude and phase. This gives access to absorption and dispersion spectroscopy. In principle, the availability of this spectral information allows different materials or

²While NMR spectroscopists do quote results in the THz range, NMR measurements on these picosecond timescales use a relaxation technique involving extrapolation, rather than a direct measurement (Marshall and Verdun 1990).

3.2 THz Imaging Horizons and Hurdles

diseases to be uniquely identified within an image. The investigation of this goal and development of algorithms towards it, form the focus of Ch. 5 of this Thesis.

T-rays can penetrate and image inside most dielectric materials, which may be opaque to visible light and low contrast to X-rays, making T-rays a useful and complementary imaging source in this context.

A goal of T-ray imaging is to produce images with component contrast enabling an analysis of the water content and composition of materials. In the medical realm such a capability presents tremendous potential to identify early changes in composition, and thereby function as a precursor to specific medical investigations and treatment. Moreover, in conventional optical transillumination techniques that use near-infrared pulses, large amounts of scattering can spatially smear out the objects to be imaged. T-ray imaging techniques, due to their longer wavelengths, can provide significantly enhanced contrast because of reduced Rayleigh scattering, which is proportional to λ^{-4} (Ciesla et al. 2000).

3.2.2 Challenges and Hurdles

Sensing and imaging with terahertz frequency radiation remains an immature technology and faces many challenges. Various factors severely constrain plausible scenarios for the application of THz technology. This section discusses the challenges facing T-ray imaging. Several of these challenges, including SNR, acquisition rate and resolution, reflect common problems encountered in a number of imaging modalities. Other challenges, such as the need for a spectroscopic database for biological tissues and other materials, are unique to THz imaging. Where appropriate, recent progress addressing these problems is highlighted and potential future research directions are described.

Water

Perhaps the most restrictive challenge facing THz imaging in many applications is the high absorption coefficients of water and other polar liquids. The absorption coefficient for liquid water is as high as 150 cm^{-1} at 1 THz. This strong absorption limits sensing and imaging in water-rich samples for most terahertz applications and prohibits transmission mode imaging through thick tissue. For this reason, current biomedical THz research has primarily focused on skin conditions (Löffler et al. 2001, Woodward

et al. 2003), and much imaging research has relied on reflection mode geometries (McClatchey et al. 2001, Dorney et al. 2002).

Power

The typical average power of an optical laser-based THz wave source is the order of a μW (from $0.1 \mu\text{W}$ to $100 \mu\text{W}$). This is due in part to low conversion efficiency. Typical conversion efficiencies for optoelectronic generation are around 10^{-6} W/W. For sensing applications with a single pixel detector, this power can provide a SNR of 10^5 or higher. However, for a detector array system for real-time 2D imaging, the available THz power is spread over multiple detectors and the dynamic range is considerably reduced (Wu et al. 1996).

Spatial Resolution

The resolution of conventional T-ray imaging systems is limited by the wavelength of the THz radiation (0.3 mm for 1 THz). This is not detailed enough for a number of applications including imaging of cellular structure. There is, therefore, widespread interest in techniques to improve the spatial resolution of T-ray imaging.

Near-field imaging can greatly improve the spatial resolution of T-ray sensing and imaging systems. Early groups used a collection mode near-field imaging technique utilising a small aperture in a metallic film to block all but a small fraction of the THz radiation (Hunsche et al. 1998). The resolution is determined by the size of the aperture, but is limited by the thickness of the metallic film, which must be thick enough to prevent leakage of THz radiation through the film. A resolution of $7 \mu\text{m}$ has been demonstrated using this technique (Mitrofanov et al. 2000, Mitrofanov et al. 2001a). The limitation of such a system is the extremely low throughput of the T-rays past the emitter tip, since the transmitted T-ray field is inversely proportional to the third power of the aperture size. It is nearly impossible to obtain a sub-micron spatial resolution with the present aperture based technologies. Temporal and spectral THz reshaping on propagation through a subwavelength aperture are an additional limitation (Mitrofanov et al. 2002), as is THz tunneling through a thin aperture screen (Mitrofanov et al. 2001c).

Recent progress in near-field THz imaging has been made via an alternate technique utilising an oscillating metal probe. The concept is adapted from scanning near-field

3.2 THz Imaging Horizons and Hurdles

optical microscopy (SNOM). A very sharp metal tip is oscillated very near to the surface of the sample in the THz beam as illustrated in Fig. 3.5(a). The metal tip interacts with the evanescent THz field over a very small area the size of the tip. A lock-in amplifier is used to measure the THz field modulation at the probe oscillation frequency. This provides a measure of the THz interaction with the sample over the very small area. This technique has recently been used to demonstrate nanometre resolutions down to 150 nm, highlighting the promise of near-field THz imaging (van der Valk and Planken 2002, Chen et al. 2003). An example THz image of 10 μm wide metallic stripes on a semi-insulating silicon substrate is shown in Fig. 3.5(b).

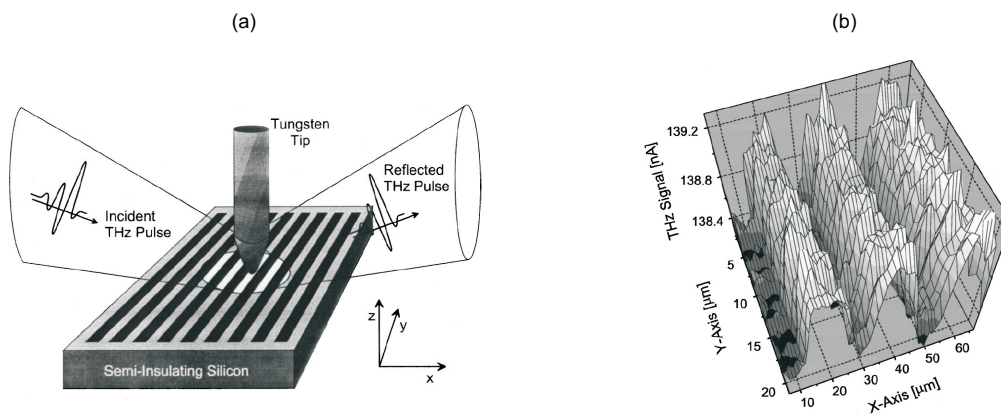


Figure 3.5. Near-field THz imaging based on SNOM. (a) The THz beam is focused onto the surface of the sample. A metallic tip is oscillated near the focal point, modulating the reflected radiation. The reflected THz pulse is detected using lock-in detection at the tip oscillation frequency. (b) A near-field THz image of a semi-insulating silicon substrate lined with 10 μm wide metallic stripes. After (Chen et al. 2003).

Another technique for near-field imaging utilises a dynamic aperture (Chen et al. 2000b, Chen and Zhang 2001). A THz beam is focused on a semiconductor wafer (GaAs or Si), which serves as a gating material. An optical pulse, synchronised with the pump and probe beams, is focused at the centre of the THz beam spot. The optical pulse creates a conducting layer at the focal point by photo-inducing free-carriers; this layer then modulates the transmitted THz beam. The spatial resolution of this method is determined by the focus size of the near-infrared laser beam and a resolution of $(\lambda/100)$ has been demonstrated. One drawback of this method is the difficulty in coating a gating material on the surface of the sample. Other potential apertureless near-field imaging techniques utilise tightly focussed optical beams to reduce the size of the generated THz beam (Yuan et al. 2002).

Another potential drawback of near-field techniques is the requirement to scan the target. This results in prohibitive acquisition times. A near-field CCD imaging technique would require advanced algorithms to deal with the problems of diffraction and has not yet been considered in the literature.

Signal-to-Noise Ratio

THz time domain spectroscopy systems are capable of providing a very high SNR of over 100,000 (van Exter and Grischkowsky 1990b). However, in imaging applications, a number of factors combine to dramatically reduce the SNR to the point where it becomes a limiting concern. Some of these factors include the need to accelerate the imaging acquisition speed and the high absorption of many materials.

Solutions to the problem of SNR are sought in improvements to the T-ray hardware. THz sources have very low average output powers and THz sensors have relatively low sensitivity compared to sources and sensors operating in the optical spectrum. Both of these aspects of T-ray systems are foci of current research and continue to improve. Other problems are related to the THz generation process, which results in THz beams that are not Gaussian and cannot be collimated as well as optical beams. This results in additional noise in THz images. Potential solutions to the SNR problem may be found in free-electron lasers (Williams 2002, Biedron et al. 2004) or in all electronic THz systems (van der Weide 1994) although currently each of these alternatives has its own disadvantages.

Acquisition Speed

Conventional THz imaging systems rely on scanning the sample in x and y dimensions to obtain an image. This places severe limits on the available acquisition speed. The first T-ray imaging system (Hu and Nuss 1995) demonstrated an acquisition rate of 12 pixels/second. Rates up to 50 pixels/second have been demonstrated (Zhao et al. 2002a), but significant advances are required to allow real-time imaging. Two-dimensional (2D) electro-optic sampling has been used together with a CCD camera to provide a dramatic increase in imaging speed (Wu et al. 1996) and rates as high as 5000 pixels/second are feasible (see Sec. 3.3.2). Unfortunately, a lock-in amplifier cannot be synchronised to multiple pixels. The relegation of the lock-in amplifier results in a significant reduction in SNR compared to the scanned approach. This may

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be partially overcome through the use of a high speed complementary metal-oxide semiconductor (CMOS) camera and software lock-in detection (Miyamaru et al. 2004).

The use of a chirped probe pulse to allow simultaneous sampling of the whole THz temporal profile (Jiang and Zhang 1998b, Jiang and Zhang 1998a) can provide a comparable imaging speed to 2D electro-optic sampling, but in addition to a reduced SNR this technique has the disadvantages of reduced frequency bandwidth and a limited temporal window (see Sec. 3.3.3). Progress in this domain is largely reliant on other technologies and improvements are expected to arise from developments such as faster galvanometric stages and lock-in CCD cameras (Spirig et al. 1995).

Limited Frequency Bandwidth and Resolution

Currently, standard photoconductive antenna (PCA) THz sources are limited to frequencies below 3 or 4 THz. Optical rectification provides a wider bandwidth – generation and detection bandwidths in excess of 30 THz have been demonstrated (Han and Zhang 1998b, Han and Zhang 1998a), however this is at the expense of THz power (and therefore SNR). Ideally a THz imaging system would allow spectroscopic responses to be measured up into the infrared. This would not only allow broader signatures to be observed but it allows the potential for reduced water attenuation, which falls dramatically as the frequency increases over 100 THz.

In addition to a high bandwidth, an ideal THz spectrometer would provide a narrow frequency resolution to enable fine spectral fingerprints of materials to be determined. THz-TDS systems provide a typical frequency resolution of 10-50 GHz. CW THz spectroscopes can offer much finer resolutions. For example, optical parametric generation of a CW THz wave provides a tunable, narrow bandwidth radiation source. With a seed idler beam from a laser diode (1.07 μm), a YAG laser at 10.6 μm generates a THz wave in a LiNbO₃ crystal (Kawase et al. 2001). The THz wavelength can be tuned from 0.7 THz to 2.4 THz, and the bandwidth is less than 2 MHz. A CW THz source may also be designed by frequency beating two semiconductor diode lasers in a photomixer; this provides a low cost, tunable THz source with very narrow bandwidth (Nahata et al. 1999). One difficulty with CW THz sources is the fact that coherent detection is not possible and incoherent detection methods must be used. These detectors generally provide lower SNR than pulsed detection techniques.

Scattering

Scattering is a common problem for many imaging modalities. In X-ray tomography scattering of X-ray photons causes artifacts in reconstruction (Herman 1980), while in optical tomography of human tissue scattering is the main transport phenomenon and reconstruction algorithms are based on modeling photon propagation as a diffusive process (Natterer and Wübbeling 2001, Markel and Schotland 2001). T-rays exhibit significantly reduced Rayleigh scattering compared to near-infrared optical frequencies due to the increased wavelength. However, scattering remains an important concern in THz sensing and imaging. The scattering of THz radiation has been investigated using Teflon spheres and scattering related dispersion was noted (Pearce and Mittleman 2001). Others have compared theoretical models of THz propagation in tissue phantoms with experimental results and shown that knowledge of the material scattering parameters is essential for accurate simulations (Walker et al. 2004). Jian et al. (2003) demonstrated the ability to characterise multiply-scattered THz waves by correlating fields measured at different positions and times.

These advances may allow the scattering process to be accurately modeled to aid the future development of diffusion imaging algorithms, such as those adopted for near-infrared imaging. Other authors have compared the scattered and ballistic THz radiation to yield additional information concerning the sample under study and have shown that this technique has promise with regard to cancer detection (Löffler et al. 2001).

Target Reconstruction

Much of the literature concerning T-ray characterisation of materials considers only transmission through thin parallel-faced samples (Duvillaret et al. 1996), or reflection from relatively flat surfaces (Mittleman et al. 1997). However, a large class of applications calls for imaging of irregularly shaped 3D objects. This presents a number of difficulties in terms of collection optics and reconstruction algorithms. Several groups have focused their attention on this problem resulting in a number of techniques and algorithms for target reconstruction (Zhang 2004). A synthetic aperture radar-based technique has been demonstrated (McClatchey et al. 2001) whereby reflection-mode images of the target are obtained at multiple angles and the 3D reflecting profile of the target is reconstructed. In addition, a bistatic THz imaging system consisting of THz receivers at multiple angles relative to the illuminating antenna has been used to image

3.2 THz Imaging Horizons and Hurdles

cylindrical reflecting structures (Dorney et al. 2001a) and irregular apertures (Ruffin et al. 2001).

This question is one of the major problems undertaken within this Thesis, Ch. 4 describes the development of several tomographic imaging systems and reconstruction algorithms for general 3D imaging.

THz Spectroscopic Database

One of the primary advantages of THz imaging over competing techniques is the availability of spectroscopic data within a potentially crucial frequency band. Unfortunately, the responses of many materials, in particular biological tissues, are unknown in this band. Work has commenced to characterise tissues, such as glucose (Nishizawa et al. 2003), RNA (Globus et al. 2003), DNA, (Smye et al. 2001, Markelz et al. 2000, Brucherseifer et al. 2001), human tissues (Fitzgerald et al. 2003) and illicit drugs such as methamphetamine (Kawase et al. 2003a). However, this remains a significant area for future research. This problem is compounded by the fact there are an enormous number of intra- and inter- molecular interactions that have an impact within this frequency regime, making interpretation of the detected spectra difficult.

An associated problem is the development of computer aided diagnostic algorithms for interpreting the multispectral images obtained by T-ray imaging. A number of authors have considered this question by fitting the measured data to linear filter models and using the filter coefficients as a means to classify gas mixtures (Mittleman et al. 1996) and tissue types (Ferguson et al. 2002a). One of the most important potential applications for terahertz technology is the detection and identification of biological and chemical agents (Woolard et al. 1999, Walker et al. 1998, Woolard et al. 2001, Brown et al. 2002).

Chapter 5 of this Thesis contributes to this body of work by developing algorithms for automated material classification, and applies these algorithms to several case studies highlighting potential applications.

Size

Current T-ray imaging systems require areas of a few square metres, most of which is dominated by the ultrafast laser as illustrated in Fig. 3.6. This size is impractical for many applications. One promising concept that has enormous potential, particularly

in biomedical imaging, is a T-ray endoscope capable of insertion within the human body. The goal of an endoscopic T-ray probe requires a number of significant advances. One enabling technology is that of the T-ray transceiver (Chen et al. 2000a, Chen et al. 2001). This technique utilises the reciprocal relationship between optical rectification and electro-optic detection to allow a single $\langle 110 \rangle$ oriented ZnTe crystal for both the emission and detection of THz pulses. In principle, such a transceiver could be made as small as 1 mm^2 and mounted at the end of an optical fibre for endoscopic applications. A PCA based transceiver with twin photoconductive dipole antennas fabricated on the same substrate has also been demonstrated (Tani et al. 2000, Tani et al. 2002).

Lai et al. (1998) demonstrated a micromachined, photoconductive terahertz emitter with a size of $0.3 \text{ mm} \times 0.3 \text{ mm}$. However, a large number of practical issues remain unresolved before an endoscopic THz imaging system may be realised. One significant problem is that of the miniaturisation of system components such as the optical chopper.

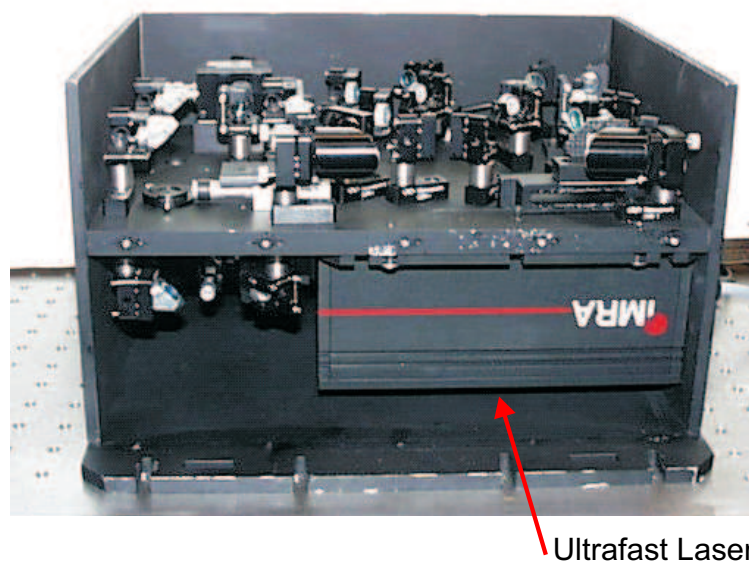


Figure 3.6. Photo of a THz imaging system. This system was designed to be semi-portable. It is mounted in a self-contained box containing the ultrafast laser and the required optics for THz-TDS. The THz imaging system has approximate dimensions of 400 mm wide 300 mm deep by 350 mm high. For reference, the distance between the mounting holes in the optical table is 1 inch (25.4 mm). After (Li et al. 1999b).

3.3 Pulsed THz Imaging Architectures

Cost

Finally, it is worth noting that the high cost of ultrafast Ti:sapphire lasers impedes THz imaging in a number of application settings. The typical cost of a T-ray sensing system and an imaging system is \$100,000 and \$200,000, respectively. This price is acceptable for academic research, but may be too high for general purpose applications. Solid-state electronic T-ray sources promise to greatly reduce the total cost in the future. Nevertheless, T-ray systems compare favourably in price with X-ray CT and NMR systems, indicating that price is not necessarily a barrier to commercialisation provided the application motivation is sufficiently strong.

Tunable continuous-wave terahertz imaging systems based on photomixing diode lasers may offer significant advantages over pulsed systems both in terms of cost and size (Gregory et al. 2004).

3.3 Pulsed THz Imaging Architectures

Pulsed THz imaging, which was coined ‘T-ray imaging’, was first demonstrated by Hu and Nuss from Bell Laboratories in 1995 (Hu and Nuss 1995). Since then a number of variations and alternatives have been developed. Terahertz imaging has been demonstrated for a wide array of applications from imaging microchips (Mittleman et al. 1996), leaf moisture content (Hadjiloucas et al. 1999), skin burn severity (Mittleman et al. 1999), tooth cavities (Knott 1999) and skin cancer (Woodward et al. 2001). Several excellent reviews of THz-TDS (Dahl et al. 1998) and T-ray imaging (Mittleman et al. 1996, Mickan et al. 2000, Chamberlain 2004) are available.

An impressive display of the ability of THz imaging to reject thermal background noise is shown in the image a burning butane flame (Fig. 3.7). A transmission architecture was used, whereby the THz radiation was transmitted through the flame and the delay of the resultant pulse was measured. The delay of the pulse is proportional to the refractive index of the air, which in turn is proportional to the temperature of the flame at that location. Hence an image indicating the spatial distribution of the flame temperature is produced (Mittleman et al. 1999).

In this Thesis, three principle THz imaging architectures are utilised. These three systems are referred to respectively as ‘traditional scanning THz imaging’ after the method of Hu and Nuss (1995), ‘two dimensional electro-optic sampling’ after Wu et

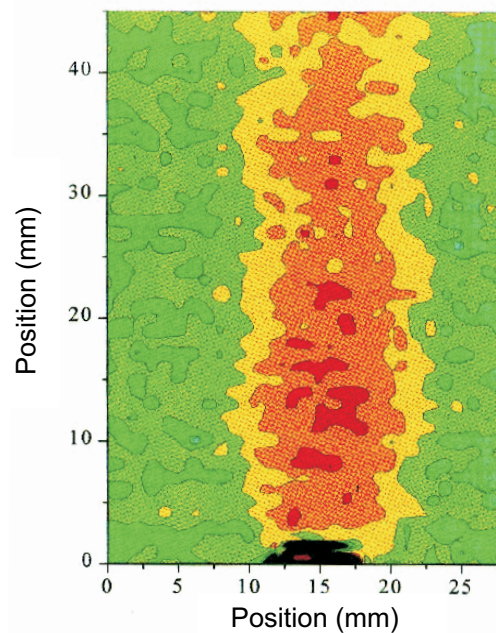


Figure 3.7. THz image of a butane flame. As the air heats up its refractive index increases. This results in increased delay of the THz pulse and allows the THz image to depict the spatial variation in temperature across the flame. In this pseudo-colour image green corresponds to lower temperature regions and red corresponds to hotter regions. After (Mittleman et al. 1999).

al. (1996) and ‘chirped probe beam imaging’ based on the principles of Jiang and Zhang (1998a). These three techniques are described in the following sections.

3.3.1 Traditional Scanning THz Imaging

Conceptually, a scanning THz imaging system is a very simple extension of a standard THz-TDS system, as described in Sec. 1.2.2. In its simplest realisation the sample mount is replaced with a 2D translation stage and the remainder of the system is unchanged. The THz spectrum is then acquired repetitively as the target is raster-scanned. This system allows the THz spectrum to be measured at every position (pixel) of the target. While this method provides extremely high SNR, in excess of 10^5 (van Exter and Grischkowsky 1990b), its disadvantage is its speed. In THz-TDS systems a lock-in amplifier (LIA) is typically used to digitise the signal. To attain a high SNR the LIA time constant is set to approximately 100 ms. This requires a settling time of 300 ms per point for accurate measurements. This results in prohibitively long acquisition times

3.3 Pulsed THz Imaging Architectures

for THz imaging experiments. For example: if a temporal resolution of 50 fs is used to acquire each THz pulse over a period of 5 ps, and a 10 cm by 10 cm image is acquired with a spatial resolution of 1 mm, this gives a total of one million samples, and a total acquisition time of 84 hours!

The LIA time constant may be reduced at the expense of SNR – however the motorised translation stages impose an additional bottleneck. A typical motion stage used in a THz-TDS system has a maximum velocity of 2 cm.s^{-1} , which imposes a minimum limit of 50 ms to move between two horizontal samples and a minimum acquisition time of 15 minutes (for the same dimensions discussed above).

In 1995 Hu and Nuss at Bell Labs proposed a number of modifications to the standard THz-TDS system to dramatically accelerate it for THz imaging applications (Hu and Nuss 1995). They used optically gated photoconductive antennas for the generation and detection of terahertz pulses. They replaced the slow translation stages with a rapid 20 Hz scanning delay line that iteratively scanned back and forth over 0.75 cm at a speed of 15 cm.s^{-1} . A digital signal processor (DSP) was utilised instead of a LIA to acquire and digitise the signal. The DSP also performed a realtime Fast Fourier Transform (FFT) on the data and displayed the image. The sample was scanned in x and y dimensions to acquire an image. This system is illustrated in Fig. 3.8 and achieved an acquisition rate of 12 pixels/s with a signal to noise ratio greater than 100:1. This system was used to image leaves, bacon and semiconductor circuits (Mittleman et al. 1996).

Experimental Setup

All the experimental results presented in this Thesis utilise a femtosecond laser consisted of a Mai Tai mode-locked Ti:sapphire laser and a Hurricane Ti:sapphire regenerative amplifier from Spectra-Physics. This laser generates near-infrared (NIR) 802 nm pulses with a pulse duration of 130 fs. The pulse energy is $700 \mu\text{J}$ at a repetition rate of 1 kHz, providing 0.7 W average power.

One of two THz emitters were used, dependent upon the desired application. For high power, low bandwidth applications a photoconductive antenna was adopted. Photoconductive antennas were manufactured by gluing two electrodes on a 0.6 mm thick GaAs wafer using conductive glue. The electrodes were biased using a direct current (DC) power supply and the bias set to ensure a strong electric field between the electrodes. The breakdown field of GaAs is 400 kV/cm, which theoretically allows a bias

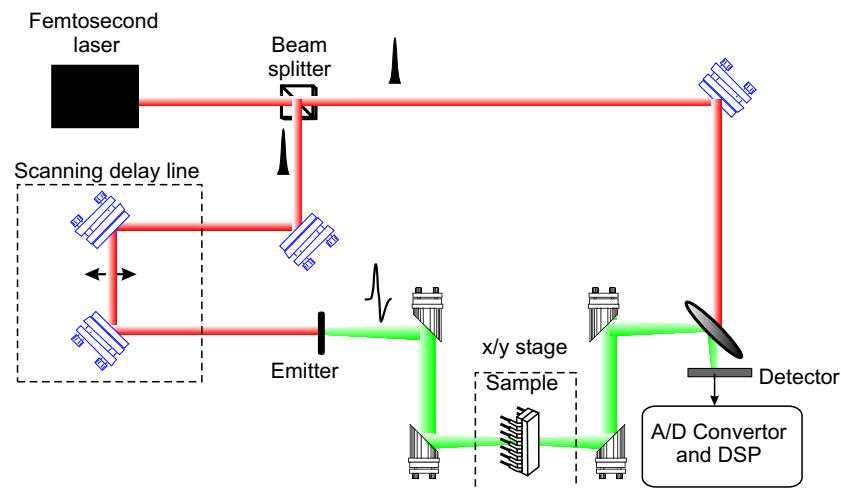


Figure 3.8. Illustration of scanned THz imaging. The galvanometric scanning delay line is scanned over a range of 0.75 cm at a rate of 20 Hz to allow an imaging speed of 20 pixels/second. The THz signal is digitised using a digital signal processor that performs the FFT of the data in real time. The image is formed by scanning the mechanical motion stages in x , y and time dimensions. After (Hu and Nuss 1995).

voltage of 624 kV for an electrode spacing of 16 mm. In practice a much lower bias of 2 kV was used, as heating of the GaAs wafer during the experiment caused arcing and breakdown to be observed at much lower fields. Hemispherical lenses are often used with PCAs to maximise the coupling of the THz field to the air in the required direction (Jepsen and Keiding 1995). This additional complexity was avoided by using widely spaced electrodes with a typical gap of 16 mm, and an unfocused laser in a topography referred to as a photoconductive planar striplines (Tani et al. 1997, Stone et al. 2002). This reduced the divergence of the emitted THz radiation and allowed the emitted THz beam to be collimated with an off-axis parabolic mirror.

When higher bandwidth THz spectroscopy was desired, and output power was less critical, optical rectification was used for generation of the THz pulses. Here, the ultrafast laser pulses were incident on a 2 mm thick $\langle 110 \rangle$ oriented ZnTe crystal. The optical rectification process is described in Sec. 2.1.1. In this case the THz power is proportional to the pump power. A pump power of 100 mW was used. The bandwidth of the THz radiation generated by OR is directly related to the pulse width, and for 130 fs pulses the THz bandwidth was approximately 2.2 THz.

Figure 3.9 shows typical THz pulses generated using the laser system and PCA and OR THz emitters. The bandwidth of the OR source is approximately two times wider,

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while the output power is 15 times lower than the PCA source. Note that the amplitude of the two signals have been normalised for clarity.

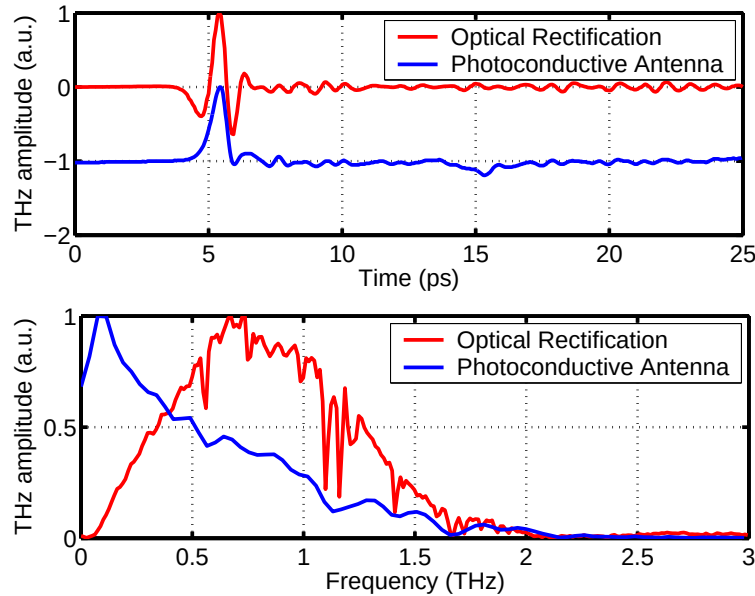


Figure 3.9. Comparison of THz pulses generated by PCA and OR emitters. (top) Time domain THz pulses generated by optical rectification and a photoconductive antenna (vertically offset and normalised for clarity). The OR source was a 2 mm thick $\langle 110 \rangle$ ZnTe crystal, and a pump power of 100 mW was used. The PCA was a GaAs wafer with electrodes separated by 16 mm at a bias voltage of 2000 V, a pump power of 20 mW was used. (bottom) THz spectrum of the two THz emitters. The difference in bandwidth and pulse shape is clearly illustrated.

A scanning THz imaging system was constructed and the experimental schematic is given in Fig. 3.10. The polarisation of the laser pulses is rotated using a half-wave plate (HWP). This determined the relative proportion of the laser pulses split into the pump and probe beams by the cubic beamsplitter and is used to adjust the pump power depending upon the THz emitter in use. The pump beam is directed onto two mirrors (M3 and M4) mounted on a translation stage that allows the propagation distance of the pump beam to be modified. The pump beam is amplitude modulated using a mechanical chopper that serves to block and transmit the pump beam at a controlled frequency. The chopper reference frequency is input into the lock-in amplifier and used for phase sensitive detection, which is discussed in Sec. 3.3.2. In general, the chopper frequency should be set as high as possible to provide maximum noise reduction, however it must also be significantly lower than the laser repetition rate (1 kHz) to avoid

aliasing effects. A chopper frequency of 144 Hz proved experimentally to be a good compromise between these two criteria.

After chopping, the pump beam is incident on the THz emitter. As the optical spot size (and hence the THz generation area) is much smaller than the THz wavelength the emitted THz radiation is sharply divergent and is collimated using an off-axis parabolic mirror, PM1. Another pair of parabolic mirrors (PM2, PM3) are used to focus the THz beam on the target and recollimate the transmitted THz field. A final parabolic mirror (PM4) is used to focus the THz radiation on the detector.

Free-space electro-optic sampling (Wu and Zhang 1995) is used for the detection of the THz electric field. The THz radiation is reflected by an indium tin oxide (ITO) beamsplitter. A thin layer of ITO is coated on a glass substrate. This provides high reflectivity for the THz beam while transmitting over 90% of the NIR optical beam. The ITO beamsplitter THz reflectivity compares well with silver coated mirrors and has high mechanical stability, unlike pellicle beamsplitters, which are subject to acoustic resonances (Bauer et al. 2002). The NIR probe beam is transmitted by the ITO glass beamsplitter and propagates collinearly through a polished 4 mm thick $\langle 110 \rangle$ ZnTe crystal. The probe beam is vertically polarised using a polariser (P1) prior to the pellicle, as it propagates through the ZnTe crystal its polarisation is rotated proportionally to the instantaneous THz electric field. ZnTe is favoured for EOS because of its physical durability, its high second order nonlinearity $\chi^{(2)}$ coefficient and its excellent phase matching properties (Rice et al. 1994). The group velocity of the 800 nm probe pulse and the phase velocity of the THz field are approximately equal in ZnTe. The birefringence of ZnTe is modified by the external THz electric field and the probe beam polarisation is rotated as a result of the EO or Pockel's effect (Wu and Zhang 1995). A second polariser P2, aligned at 90° to the initial polariser, modifies the amplitude of the probe pulse according to the polarisation. This signal is detected using a photodetector PD and digitised by a LIA. THz-TDS experiments more commonly employ a quarter wave bias and balanced photodetection than the crossed polariser method described here (see Sec. 3.3.2 for more details). A crossed polariser geometry was adopted to allow the system to be easily converted to alternate imaging systems as discussed in future sections.

This system measures the instantaneous THz electric field. By iteratively reducing the pump path length using the delay translation stage, the electric field at later times was measured and the temporal THz pulse profile recorded. To acquire an image,

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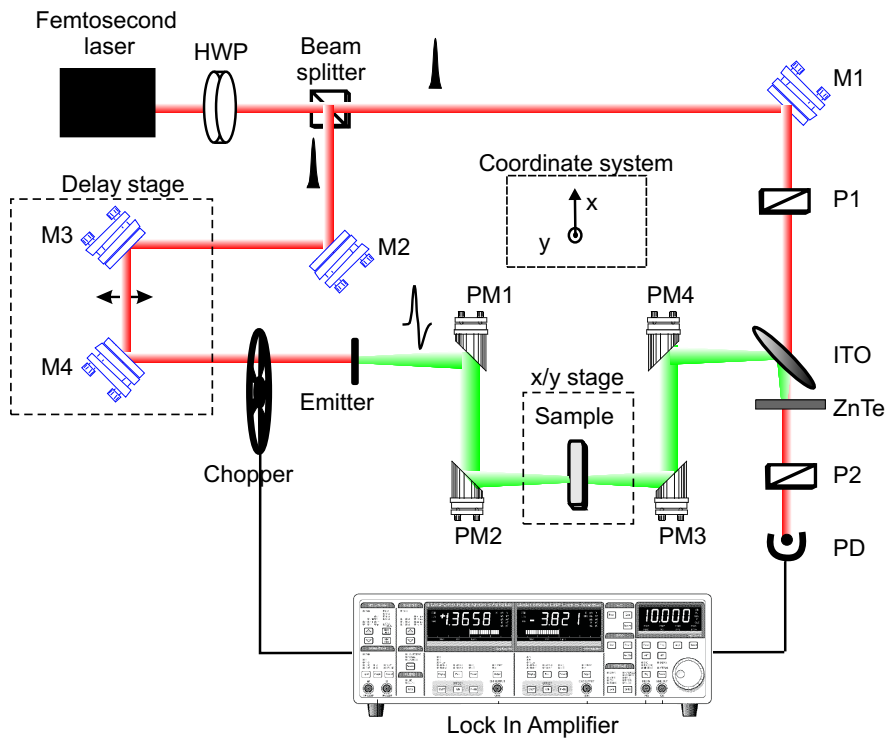


Figure 3.10. Hardware schematic for scanned THz imaging. Femtosecond laser pulses are split into pump and probe beams by a cubic beamsplitter. The pump beam path length is controlled by mirrors M3 and M4 mounted on a translation stage. After chopping, the pump beam is incident on the THz emitter (as described in the text) and generates THz pulses. The THz beam is collimated and focused on the sample by gold coated parabolic mirrors PM1 and PM2. The transmitted radiation is recollimated and focused on the detector by parabolic mirrors PM3 and PM4. The THz beam is reflected by an ITO glass THz mirror while the probe beam is transmitted, allowing both beams to propagate through the ZnTe THz detector collinearly. Polarisers P1 and P2 are perpendicular to each other. The probe beam is detected using a photodetector PD and digitised using a LIA. Inset: The coordinate system is shown. The y axis is out of the page, perpendicular to the plane of the optical table.

the pulse measurement procedure is repeated as the target is raster scanned using x and y translation stages. This system is slow, but acquires images with a very high SNR. Using a LIA time constant of 10 ms and averaging for 30 ms at each sample, the system SNR is over 1000. Using these parameters the acquisition time for a typical 50×50 pixel image with 100 temporal samples is approximately 2 hours.

Example Images

A large number of groups have used these imaging systems for a broad array of applications. The two areas of greatest interest have been in semiconductor characterisation and biomedical imaging. As an example, this imaging system was used to image an insect on an oak leaf. The target was imaged using a spatial resolution step of 0.5 mm and 300 temporal samples. Representative THz waveforms after transmission through the three major media in the image are shown in Fig. 3.11. The SNR of the free air response is greater than 1000. A THz image was produced by Fourier transforming the measured responses and imaging the Fourier amplitude of the response at each pixel for a frequency of 1 THz. This image is presented in Fig. 3.12. Scanned THz imaging provides very high image quality but long acquisition times.

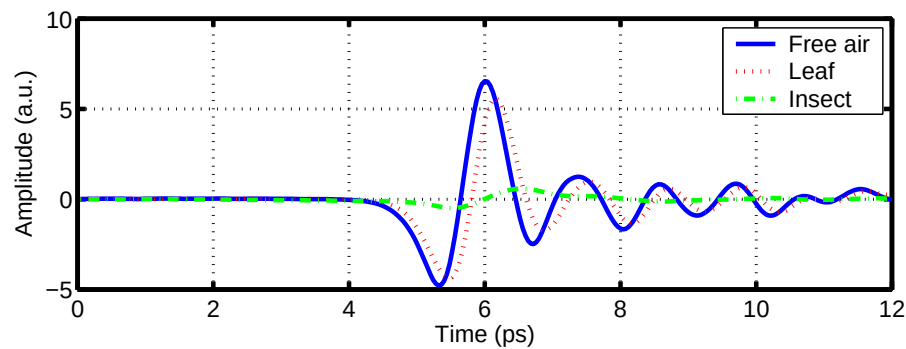


Figure 3.11. THz response obtained using a scanned THz imaging system. An oak leaf and insect were imaged using the scanned THz imaging system shown in Fig. 3.10. A $100 \times 100 \times 300$ sample image was obtained (Fig. 3.12), corresponding to $x \times y \times \text{time}$ samples; the total acquisition time was over 20 hours. The temporal responses for three pixels are shown.

3.3.2 Two Dimensional Free Space EO Sampling

Shortly after the development of scanned THz imaging systems a dramatic improvement in acquisition speed was made using two-dimensional electro-optic detection of the terahertz pulse (Wu et al. 1996). This technique provided a parallel detection capability and removed the need to scan the target. This method is based on electro-optic sampling, which was introduced in Sec. 2.2. Rather than focusing the THz pulse on the sample, quasi-plane wave illumination is used. The probe beam is expanded to a diameter greater than that of the THz beam and the two pulses are incident on the EO

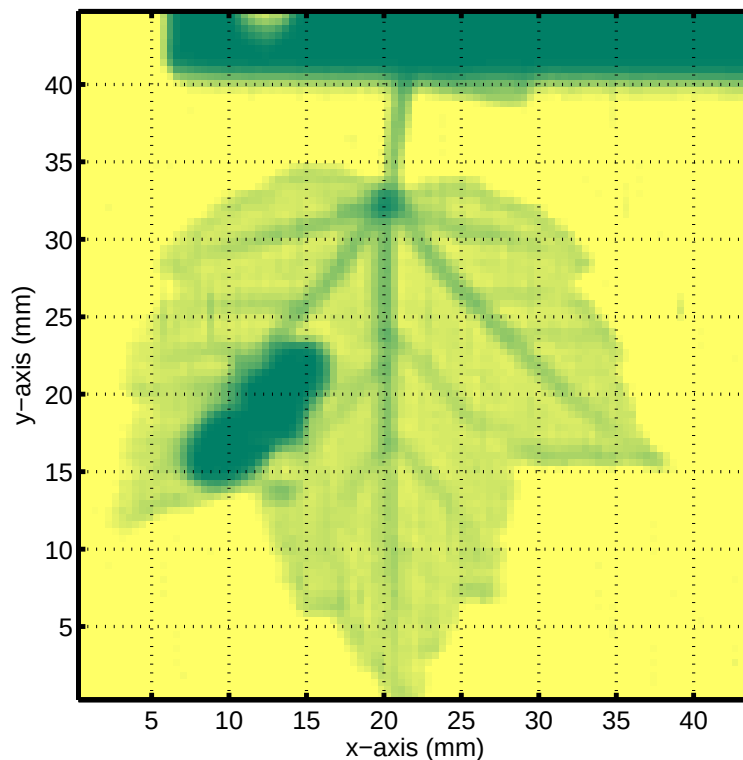


Figure 3.12. Scanned THz image of an oak leaf. The image was produced by Fourier transforming the THz temporal responses at each pixel and plotting the amplitude of each response at 1 THz. Data courtesy of X.-C. Zhang.

detector crystal. The terahertz pulse acts as a transient bias on a $\langle 110 \rangle$ oriented ZnTe crystal, inducing a polarisation in the crystal. The probe beam is then modulated by the polarisation-induced birefringence of the ZnTe crystal via the Pockel's effect. The two-dimensional (2D) THz field distribution is then converted to a 2D intensity modulation on the optical probe beam after it passes through a crossed polariser (analyser). A digital charge coupled device (CCD) camera is used to record the optical image. This system is illustrated in Fig. 3.13.

EO Sampling Near the Zero Optical Transmission Point

It was noted by Wu et al. (1996) and Jiang et al. (1999), that the standard quarter-wave bias, typically employed in THz EO detection, is suboptimal for a crossed polariser detection geometry. The typical balanced photodetector geometry is shown in Fig. 2.3, while the crossed polariser geometry is shown in Fig. 3.14. Both of these techniques may be employed to detect the polarisation modulation on the optical probe beam.

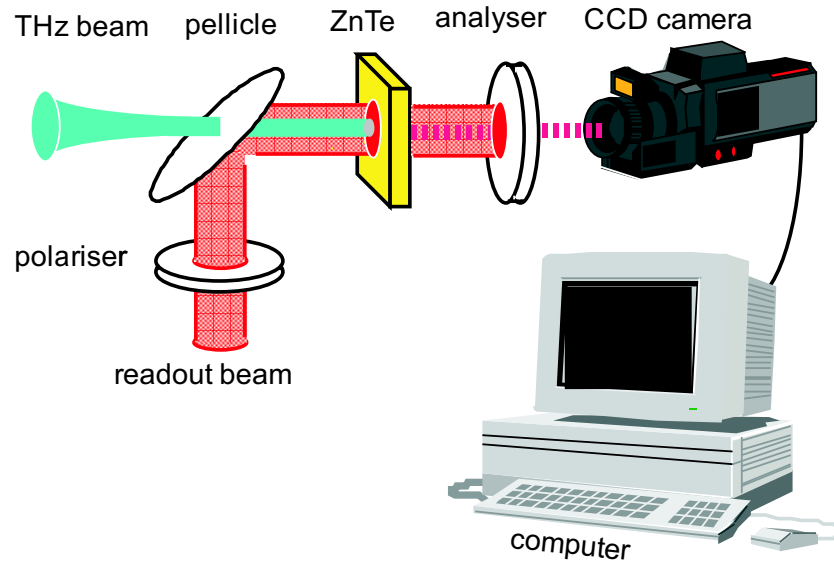


Figure 3.13. Illustration of all-optical 2D THz imaging. The image is formed by expanding the THz and probe beams and using the Pockel's effect and crossed polarisers to convert the THz field to an intensity modulation that is measured using the CCD. After (Wu et al. 1996).

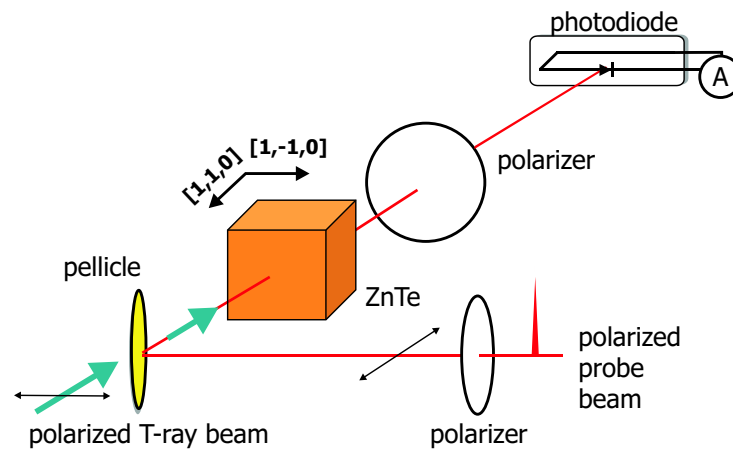


Figure 3.14. Crossed polariser EO sampling geometry. The probe pulse is linearly polarised by the first polariser before the EO crystal. Its polarisation is then modified by the Pockel's effect, depending on the instantaneous THz electric field. The second polariser is set at approximately 90° to the initial one, thereby minimising the leakage of the probe pulse in the absence of a modulating THz field.

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The balanced detection method generally applies a quarter-wave bias to the probe beam (Smith et al. 1988). This maximises both the modulated light intensity and the linearity of the Pockel's cell. The transmitted light intensity, I , observed by the photodiodes in Fig. 2.3 is given by

$$I = I_0[\eta + \sin^2(\Gamma_0 + \Gamma)], \quad (3.2)$$

where I_0 is the incident light intensity, η is a scattering coefficient, Γ_0 is the bias of the probe beam, and Γ is the THz electric field induced birefringence contribution (Jiang et al. 1999, Yariv 1991). For the balanced detection geometry shown in Fig. 3.14, the scattering component is canceled and Γ_0 is set to approximately $\pi/4$ with the quarter wave plate. It can be seen that for $\Gamma \ll \Gamma_0$, which is always true for typical THz field amplitudes, the balanced output intensity is approximately proportional to Γ . However, when a CCD is used, balanced (or differential) detection is not possible and in this case the background intensity caused by $\Gamma_0 = \pi/4$ can saturate the CCD. In addition the shot noise, which is proportional to the background light, is much larger than the contribution of the THz modulation, Γ , and greatly degrades the image SNR. For non-balanced detection (Fig. 3.14) the SNR is proportional to the *modulation depth*, which is defined as

$$\gamma \doteq \frac{I_{\Gamma} - I_{\Gamma=0}}{I_{\Gamma} + I_{\Gamma=0}}. \quad (3.3)$$

It is obvious from this definition, Eq. (3.3), that the modulation depth is maximised by setting $I_{\Gamma=0} = 0$. It appears that the crossed polariser architecture shown in Fig. 3.14 achieves this, however in practice the EO crystal has a residual birefringence, which contributes to Γ_0 , therefore to achieve zero optical transmission requires the addition of an extra compensator set to cancel the residual birefringence (Jiang et al. 1999). For the crossed polarisers architecture both $|\Gamma_0| \ll 1$ and $|\Gamma| \ll 1$, as a result Eq. (3.2) can be approximated by

$$I = I_0[\eta + (\Gamma_0 + \Gamma)^2], \quad (3.4)$$

the background light intensity I_b (the intensity measured by a photodiode) and the signal I_s (the intensity measured by a photodiode connected to a LIA) are then given by

$$I_b = I_0(\eta + \Gamma_0^2), \quad (3.5)$$

$$I_s = I_0(2\Gamma\Gamma_0 + \Gamma^2), \quad (3.6)$$

and the modulation depth becomes

$$\gamma = \frac{2\Gamma_0\Gamma + \Gamma^2}{2\eta + \Gamma_0^2 + (\Gamma_0 + \Gamma)^2}. \quad (3.7)$$

We can use Eq. (3.7) to determine the optimal value of Γ_0 to maximise γ and hence the SNR. However, for $\Gamma_0 = 0$ the measured signal is no longer proportional to Γ but is proportional to Γ^2 . This causes a number of difficulties, as the measured signals must then be distortion corrected to recover the THz electric field. To avoid this additional processing complication the compensator was omitted and the residual birefringence was $\Gamma_0 \approx 10^{-2} \gg \Gamma \approx 10^{-4}$, which remained in the linear regime. This results in a slightly degraded modulation depth and SNR compared to a compensated system.

Dynamic Subtraction

Jiang et al. (2000b) introduced dynamic subtraction to THz imaging systems as a means to dramatically improve the SNR of the images. The major source of noise in THz pump-probe experiments is caused by the amplitude fluctuations in the ultrafast laser source. This noise is characterised by long term drift and is described as $1/f$ noise (Milotti 1995).

For this reason THz-TDS experiments typically employ a LIA to allow phase sensitive detection of the THz field. Without an LIA, the long term amplitude drift in the laser power greatly reduces the SNR of the measurements. A mechanical chopper is used to modulate the THz beam, the LIA is then synchronised to this modulation (chopper) frequency and detects the relative difference in the amplitude of the signal with the THz beam on and off. Due to the $1/f$ characteristic of the laser noise, the higher the chopper frequency the lower the noise in the LIA output.

A CCD with a LIA at each pixel has been proposed (Wu et al. 1996) but has not yet been demonstrated. In order to utilise phase sensitive detection with a 2D FSEOS system Jiang and colleagues implemented a *dynamic subtraction* technique. In this method, as illustrated in Fig. 3.15, the CCD is set to trigger at a fixed sample rate, the trigger out signal from the CCD is then taken as the input to a frequency divider circuit, which halves the frequency, and this signal is used to trigger the chopper.

3.3 Pulsed THz Imaging Architectures

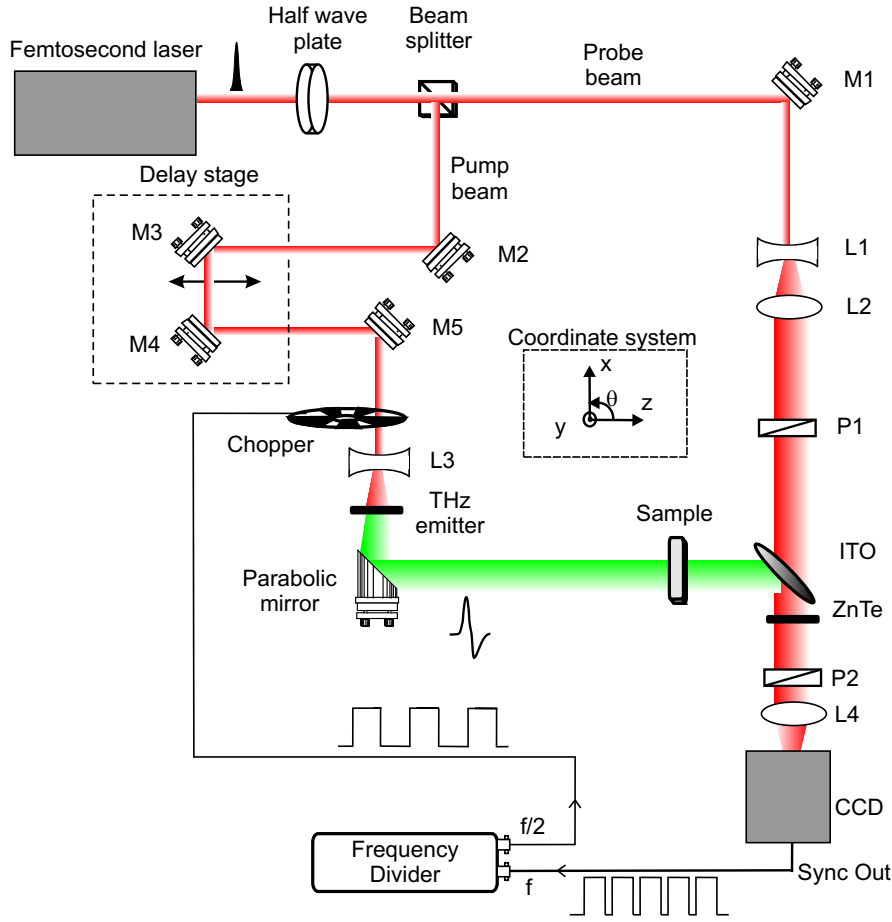


Figure 3.15. Schematic of terahertz imaging with dynamic subtraction. A mechanical chopper modulates the THz pulse. The control signal for the chopper is derived from the sync out signal from the CCD camera, following a frequency divider circuit that halves the frequency. The remainder of the imaging system is described in detail in Fig. 3.16.

For example, with a CCD frame rate of 30 frames per second (fps) the THz signal would be amplitude modulated at a frequency of 15 Hz. The chopper provides a 50% duty cycle and therefore every second frame measures the THz signal amplitude, while every other frame simply measures the probe laser power without the THz field. This corresponds to the background noise. Every second frame is subtracted from the previous one and thereby the laser background noise is subtracted from each frame to compensate for the long term background drift. Typically multiple frames are averaged to further improve the SNR and the output signal is calculated according to

$$S = \frac{\sum_{n=1}^N (I_{2n} - I_{2n-1})}{\sum_{n=1}^N (I_{2n} + I_{2n-1})}, \quad (3.8)$$

where N is the number of accumulated frames and I_n is the measured CCD intensity at time $n\delta t$ given a frame sampling period of δt .

Synchronised Dynamic Subtraction

Dynamic subtraction works well for systems where the laser repetition rate is several orders greater than the CCD sampling rate. However, the Hurricane laser system used in this Thesis has a repetition rate of only 1 kHz. Deriving the chopper frequency from the CCD internal frame rate clock therefore resulted in significant phase noise in the signal. If the laser timing and the CCD timing are not accurately synchronised, some CCD frames will accumulate more laser pulses than others and this will result in a significant reduction in SNR. To overcome this problem a synchronised dynamic subtraction technique was developed to synchronise the chopper and CCD to the laser timing reference. This is schematically illustrated in Fig. 3.16.

The trigger-out signal from the laser is synchronised with the laser pulses at a frequency of 1 kHz. A frequency divider circuit generates $f/32$ and $f/64$ subharmonics of this 1 kHz signal and these are used to trigger the CCD and the chopper respectively. These signals are illustrated in Fig. 3.17. The CCD trigger signal was chosen to approximate the maximum frame-rate of the CCD given its frame transfer period of 15 ms.

To illustrate the equivalence between this dynamic subtraction method and lock-in detection we consider the following expression for the measured image, S , when N differential frames are averaged,

$$\begin{aligned}
 S &= \sum_{n=0}^N I(n.\delta t)(-1)^n, \\
 &= \sum_{n=0}^N I(n.\delta t) \exp(-i\frac{2\pi n}{2\delta t}\delta t), \\
 &= \text{DFT}[I(t)]_{f=f_o/2},
 \end{aligned} \tag{3.9}$$

where f_o is the image acquisition frequency given by the inverse of the sampling period, δt , $i = \sqrt{-1}$ and DFT denotes the Discrete Fourier Transform (DFT). Thus the signal S is the portion of the measured intensity that is modulated at the chopper frequency $f_o/2$. This is equivalent to the function of a LIA, which detects the signal at the chopper modulation frequency (a LIA normally samples much faster than the desired detection frequency). The synchronised dynamic subtraction method maximises

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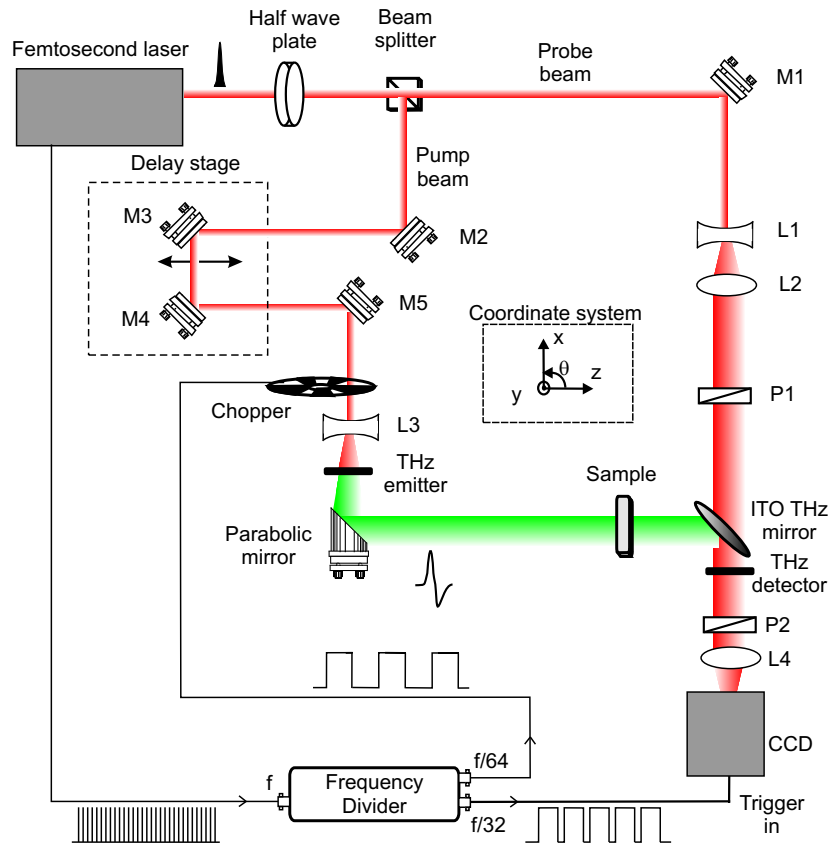


Figure 3.16. Schematic of 2D FSEOS terahertz imaging with synchronised dynamic subtraction. A mechanical chopper modulates the THz pulse. The control signals for the chopper and the CCD are derived from the sync out signal from the ultrafast laser. A frequency divider circuit is used to generate $f/32$ and $f/64$ Hz pulses, where f is the repetition rate of the laser (1 kHz). Ultrafast laser pulses are split into pump and probe beams using a polarising cubic beamsplitter. The pump beam is reflected by mirrors M3 and M4, which are mounted on a translation stage to allow the relative path length of the pump and probe beams to be modified. The pump beam is chopped and then transmitted through a concave lens L3 onto the THz emitter to form a divergent THz beam. The THz beam is collimated using a parabolic mirror and transmitted through the target sample. The transmitted THz beam is reflected by an ITO coated THz mirror such that it propagates colinearly with the probe beam, which is expanded by the telescope lens system (L1 and L2) and polarised by polariser P1. The THz and probe beams propagate colinearly through a 4 mm thick, 2 cm diameter <110> ZnTe detector crystal. The crossed polariser P2 converts the polarisation of the probe beam to an amplitude modulation, which is focused on the CCD camera with lens L4. Inset: The coordinate system is shown.

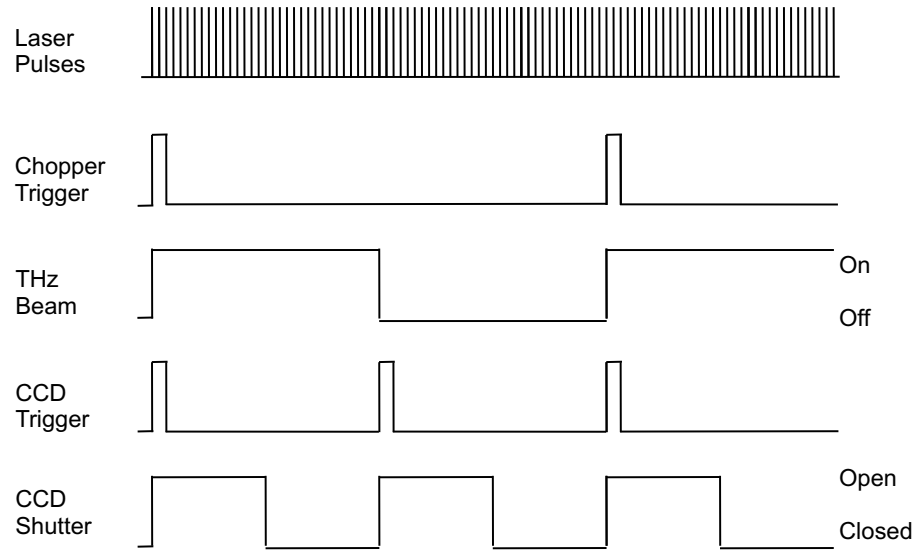


Figure 3.17. Control signals for synchronised dynamic subtraction. The control signal for the chopper is a pulse at $1/64$ of the laser repetition rate. The THz beam is modulated with a 50% duty cycle. The CCD trigger is a pulse at $1/32$ of the laser repetition rate. In this way every second frame captures the background without the THz beam present.

the SNR by modulating the signal at the highest possible frequency given the CCD's frame rate.

Sensor Calibration

Synchronised dynamic subtraction allows the THz modulated optical field to be measured with high accuracy. However a true image of the target is only obtained in the ideal case where the probe beam I_0 , the residual birefringence of the sensor crystal Γ_0 and the incident THz field (in the absence of a target) are all independent of sensor position. In practice all of these parameters vary. Equation (3.6) shows that the measured optical signal at each pixel is dependent upon both the THz modulating field Γ and the residual birefringence of the crystal, Γ_0 . The residual birefringence is not constant over the sensor but is a function of position. Therefore different pixels in the image incur multiplicative noise from Γ_0 (Jiang and Zhang 1999). Assuming $\Gamma \ll \Gamma_0$, Eq. (3.6) becomes

$$I_s \approx 2I_0\Gamma\Gamma_0. \quad (3.10)$$

The measured image I_s can be corrected for the spatial variations by measuring the THz image without a sample in place and performing a deconvolution similar to that

3.3 Pulsed THz Imaging Architectures

normally performed in the frequency domain – this time performed on a pixel by pixel basis. This calibration correction for I_s is given by

$$I_{s \text{ cal}} = \frac{I_s}{I_{\text{pk (no sample)}}}, \quad (3.11)$$

where $I_{\text{pk (no sample)}}$ is the peak measured signal intensity when the THz field is applied without a sample in place. Both I_s and $I_{\text{pk (no sample)}}$ are functions of position and the correction is applied on a pixel by pixel basis.

In practice an additional calibration step was added to Eq. (3.11). Due to damage and impurities in the sensor crystal, several regions had high optical attenuation. At these pixels $I_{\text{pk (no sample)}}$ was very small and the division in Eq. (3.11) resulted in amplification of the noise. A regularisation step was added such that Eq. (3.11) was only applied at pixels where $I_{\text{pk (no sample)}}$ was greater than 10% of the maximum $I_{\text{pk (no sample)}}$ amplitude.

Figure 3.18 illustrates the improvement provided by both synchronised dynamic subtraction and the sensor calibration procedure outlined above. The 2D FSEOS imaging system described in Fig. 3.16 was used to image a 2 mm thick vertical polystyrene cylinder, which was placed in the centre of the THz beam 2 cm from the sensor crystal. Initially dynamic subtraction processing was not performed. The peak of the resultant THz pulses formed the image shown in Fig. 3.18(a). The image is noisy and the effects of the cylinder are not visible. A frame rate of 67 fps was used and 100 frames were averaged together. Next, the same target was imaged using synchronised dynamic subtraction. Again a frame rate of 67 fps was used and 100 frames were averaged to yield the image shown in Fig. 3.18(b). The noise is visibly reduced. To apply the calibration correction discussed above the sample was removed and the resultant THz image was measured. The peaks of the THz pulses at each pixel resulted in Fig. 3.18(c). Equation (3.11) was applied using the data shown in Fig. 3.18(b) and (c) and the result is shown in Fig. 3.18(d). Here the diffraction pattern caused by the polyethylene cylinder is clearly visible. The width of the cylinder in the image is much greater than the width of the actual target. This is a result of diffraction effects, which are discussed in detail in Sec. 4.5.

Recently Usami et al. (2003) demonstrated 2D FSEOS imaging using polarity modulation of the THz field rather than the optical chopping technique employed in this Thesis. Polarity modulation, when combined with dynamic subtraction was shown to improve both the modulation efficiency and the signal linearity with the THz field.

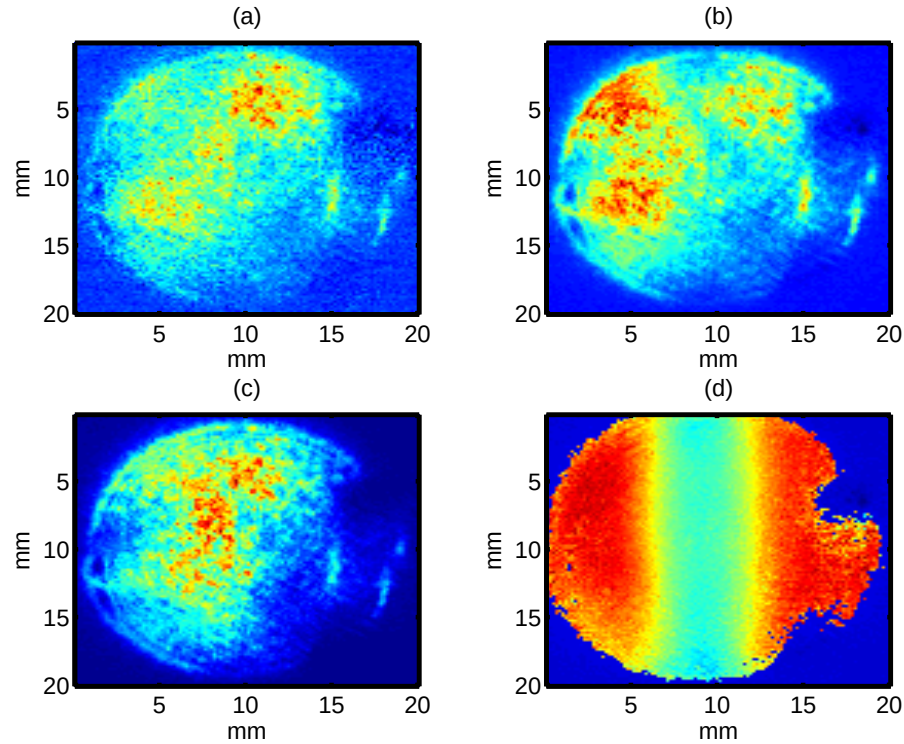


Figure 3.18. Processing stages applied to 2D FSEOS images. The 2D FSEOS THz imaging system was used to image a thin vertical polyethylene cylinder placed 2 cm from the sensor crystal. (a) A raw THz image plotted using the peak of the THz pulse at each pixel. No dynamic subtraction techniques were applied and no data correction schemes have been applied. (b) The same target was imaged using the same system using synchronised dynamic subtraction. No data correction is applied. The noise in the image is visibly reduced however the target is still not discernible. (c) The imaging system was characterised by removing the target and measuring the peak THz response at each pixel $I_{pk \text{ (no sample)}}$. This image is used to apply the data correction of Eq. (3.11). (d) Final image of the cylinder. The data in (b) was processed using Eq. (3.11) and the peak data in (c). The peak of the processed THz pulse is plotted at each pixel. The vertical cylinder is now visible. In all the subfigures, dark blue corresponds to the minimum signal intensity and increasing intensity is indicated by the colours green, yellow and orange, with red indicating maximum signal intensity.

Experimental Setup

The experimental system for 2D FSEOS THz imaging is depicted in Fig. 3.16. The regeneratively amplified Ti:sapphire laser described in Sec. 3.3.1 is used to generate 130 fs laser pulses. The laser pulses are split into pump and probe beams using a polarising cubic beamsplitter. A half-wave plate allows the polarisation of the laser to be rotated, which in turn allows the relative power in the pump and probe beams to be controlled. The pump beam is expanded using a negative lens L3 and is incident on the THz emitter. Two alternate THz emitters were used depending upon the desired application. These included a optical rectification source consisting of a 2 mm thick, 1 cm diameter $\langle 110 \rangle$ ZnTe electro-optic crystal. For this emitter, a pump power of 100 mW was used as a compromise between increasing the output THz power and risk of damaging the ZnTe crystal. This source provided an output power of approximately $4 \mu\text{W}$ and a bandwidth of approximately 2.2 THz. A photoconductive antenna source was also used for high power applications, for instance, when high SNR was required, or a strongly attenuating target was to be imaged. The PCA source consisted of a 0.6 mm thick, 3 cm diameter GaAs wafer, with metal electrodes separated by 2 cm, biased at 2 kV. A pump power of 50 mW was used. Higher pump powers were found to cause an excess of free carriers in the GaAs and resulted in screening of the bias field by the carrier field and a reduction in the output THz power (Rodriguez and Taylor 1996).

The generated THz power is collimated using a 90° off-axis parabolic mirror. The collimated THz beam illuminates the target sample. On transmission through the sample the THz radiation is reflected by an ITO THz mirror. The probe beam is expanded by a telescope beam expander consisting of negative lens L1 and positive lens L2 to a beam waist ($1/e$) of 2.5 cm. After the ITO mirror the expanded probe beam and the THz beam propagate collinearly through a 4 mm thick, 2 cm diameter $\langle 110 \rangle$ ZnTe crystal. As a result of the collinear propagation, and the phase matching conditions in ZnTe, the THz electric field spatially modulates the polarisation of the probe pulse. The probe pulse is linearly polarised by P1 and the polarisation modulation is converted to an amplitude modulation by polariser P2 whose polarisation is perpendicular to P1. The probe signal is then focused on the CCD array by L4.

The camera was a Princeton Instruments EEV576 $\times$ 384 CCD camera. It is air-cooled to -30°C to provide high sensitivity and minimise dark current. The CCD pixel size

is $22 \times 22 \mu\text{m}^2$. Typically several pixels are binned together to reduce the computational load. However, for the diffraction tomography system discussed in Sec. 4.5 it is desirable to sample the THz electric field with sub-wavelength resolution. The CCD provides very high dynamic range (12 bit) and sensitivity. CCD images are acquired on a computer where the processing stages involved in synchronised dynamic subtraction (see Sec. 3.3.2) are applied. Typically a frame rate of 67 fps was used and 100 frames were averaged to provide high SNR.

A computer acquires the image data from the CCD and controls the delay stage to allow the temporal THz waveform to be acquired at each pixel. This allows a typical image with 100 temporal steps to be acquired in 5 minutes.

3.3.3 THz Imaging with a Chirped Probe Pulse

The third imaging technique utilised in this Thesis is based on EO detection of terahertz pulses using a chirped probe pulse. This imaging technique has the highest theoretical acquisition rate of the three methods discussed, however it also has a number of inherent disadvantages. This work represented the first use of this imaging technique for transmission mode THz imaging of objects. Previous work had focused on imaging the THz beam profile (Jiang and Zhang 1998c), and other authors have used the same technique for characterising electron pulses (Wilke et al. 2002).

Electro-optic (EO) detection of a terahertz pulse using a chirped probe pulse was first demonstrated by Jiang and Zhang (1998a). This novel technique allows the full THz waveform to be measured simultaneously rather than requiring a stepped motion stage to scan the temporal profile. This provides a significant reduction in the acquisition time and greatly extends the applicability of THz systems in situations where the sample is dynamic or moving. Indeed, single shot measurements have been demonstrated for measuring a THz pulse using a single femtosecond light pulse (Jiang and Zhang 1998c).

Terahertz measurement using a chirped probe pulse is based on EO sampling (Wu and Zhang 1995), which is widely used for THz detection because of its wide bandwidth and sensitivity. In normal THz-TDS (as described in Sec. 1.2.2) the femtosecond laser pulse is used to probe the instantaneous THz field at a certain time delay; the relative delay between the probe pulse and the THz pulse is then adjusted and the measurement repeated. In this way the full temporal profile of the THz pulse is measured.

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This process can be greatly accelerated by applying a linear chirp to the probe pulse. This is done using a diffraction grating as shown in Fig. 3.19. The different wavelength components of the incident pulse traverse different path lengths due to the variation in first order diffraction angle with wavelength, λ . The output from the grating is a pulse with a longer pulse duration and a wavelength that varies linearly with time.

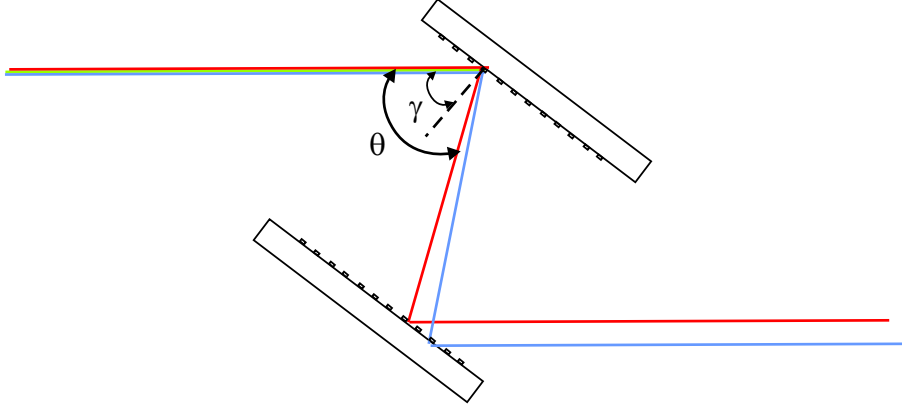


Figure 3.19. The geometry of a diffraction grating. The grating is used to impart a linear chirp to a laser pulse. The optical path length is greater for longer wavelengths. The angle of incidence is γ and θ is the angle between incident and diffracted rays.

For first order diffraction the angles of incidence and diffraction can be related by

$$d \sin \gamma + d \sin(\gamma - \theta) = \lambda, \quad (3.12)$$

where γ is the angle of incidence, θ is the angle between incident and diffracted rays, λ is the wavelength of the light and d is the grating constant. Following the conventions of Treacy (1969) if G is the perpendicular distance between the gratings, then b , the slant distance is

$$b = G \sec(\gamma - \theta), \quad (3.13)$$

and the ray path, p , is

$$p = b(1 + \cos \theta) = c\tau, \quad (3.14)$$

where τ is the group delay.

By differentiation it can be shown that

$$\delta\tau = \frac{b(\lambda/d)\delta\lambda}{cd[1 - (\lambda/d - \sin \gamma)^2]}. \quad (3.15)$$

In this way the angle of incidence and the grating separation can be varied to provide a variable chirp rate and corresponding chirped pulse width.

In EO detection this chirped probe pulse is modulated by a THz pulse. In traditional EO sampling, a 100-fs optical pulse is modulated by a short temporal portion of the THz pulse. Conceptually the chirped probe pulse can be seen as a succession of short pulses each with a different wavelength. Each of these wavelength components encodes a different portion of the THz pulse.

A spectrometer spatially separates the different wavelength components and thus reveals the temporal THz pulse. The spatial signal output from the spectrometer is measured using a CCD. This technique derives from real time picosecond optical oscilloscopes (Galvanauskas et al. 1992, Jiang and Zhang 1998a).

For maximum image acquisition speed the THz pulse and probe pulse may be expanded in the vertical dimension using cylindrical lenses. The CCD is then able to capture both the THz temporal waveforms and several hundred vertical pixels simultaneously (Jiang and Zhang 1998a) and only a single translation stage is required for spectroscopic image acquisition. This method combines the advantages of the chirped probe imaging technique with multi-dimensional electro-optic sampling as discussed in Sec. 3.3.2. However, this method degrades the SNR by spreading the available THz power over multiple pixels and diffraction effects can corrupt the temporal measurements. To avoid these additional concerns, this Thesis concentrates on the use of scanned imaging by focusing the THz pulses to a point and raster scanning the target.

Mathematical Model

Electro-optic detection with crossed polarisers imparts an amplitude modulation on the probe pulse. For relatively small modulation depths this modulation is linear and the modulated signal, $f_m(t)$, is given by

$$f_m(t) = f_c(t) [1 + kE(t - \tau)], \quad (3.16)$$

where $f_c(t)$ is the chirped probe pulse, k is the modulation constant, $E(t)$ is the THz electric field and τ is the relative time delay between the probe and THz pulse.

The spectrometer grating spatially disperses the different spectral components of the input signal. The signal detected at the CCD corresponding to a given frequency, $M(\omega_1)$, is given by the convolution of the spectral response function of the spectrometer grating, $g(\omega)$, with the square of the Fourier transform of the input signal, $f_m(t)$ (Sun et al. 1998)

$$M(\omega_1) \propto \int_{-\infty}^{\infty} g(\omega_1 - \omega) \left| \int_{-\infty}^{\infty} f_m(t) \exp(i\omega t) dt \right|^2 d\omega. \quad (3.17)$$

3.3 Pulsed THz Imaging Architectures

The normalised differential intensity, $N(\omega_1)$, is then defined as

$$N(\omega_1) = \frac{M(\omega_1)|_{\text{THz on}} - M(\omega_1)|_{\text{THz off}}}{M(\omega_1)|_{\text{THz off}}}. \quad (3.18)$$

Following Sun et al. (1998) and applying the method of stationary phase and considering the first order of k , yields

$$N(\omega_1) = \frac{\int_{-\infty}^{\infty} g(\omega_1 - \omega) 2kE(t_\omega - \tau) \exp(-2t_\omega^2/T_c^2) d\omega}{\int_{-\infty}^{\infty} g(\omega_1 - \omega) \exp(-2t_\omega^2/T_c^2) d\omega} \quad (3.19)$$

where $f_c(t)$ has been assumed to be of the form

$$f_c(t) = \exp\left(-\frac{t^2}{T_0^2} - i\alpha t^2 - i\omega_0 t\right), \quad (3.20)$$

and T_c is the chirped pulse duration, T_0 is the original laser pulse duration and α is the chirp rate in Hz/second. The frequency measured by the CCD pixel is linked to the THz temporal dimension via t_ω

$$t_\omega = \frac{\omega_0 - \omega}{2\alpha}, \quad (3.21)$$

where ω_0 is the centre frequency of the probe beam, and 2α is the chirp rate. For an ideal spectrometer with $g(\omega_1 - \omega) \approx \delta(\omega_1 - \omega)$ we see that $N(\omega_1) \propto 2kE(t_{\omega_1} - \tau)$ and $N(\omega_1)$ is linearly proportional to the amplitude of the THz pulse, with the variable ω_1 proportional to the time, t . However in most practical situations the THz signal is frequency band limited, which corresponds to a broadening of the temporal pulse.

Previous analysis (Sun et al. 1998) has shown that, given certain approximations, the temporal resolution, $T_{\min}$ is given as a function of the original optical pulse width, T_0 , and the chirped pulse width, T_c ,

$$T_{\min} = \sqrt{T_0 T_c}. \quad (3.22)$$

Assuming that the spectrometer response function, $g(\omega)$ is a Gaussian of the form

$$g(\omega) = \exp\left(-\frac{\omega^2}{\Delta\omega_s^2}\right), \quad (3.23)$$

where $\Delta\omega_s$ is the spectral resolution. The numerator of Equation (3.19) consists of two exponential terms multiplied by the THz signal. By substituting from Eq. (3.21) the

exponential terms can both be expressed in terms of ω and a simple change of variable yields a numerator of

$$\int_{-\infty}^{\infty} \exp\left(-\frac{(\omega_1 + \omega_0 - \omega)^2}{\Delta\omega_s^2}\right) 2kE(\omega) \exp\left(\frac{-2\omega^2}{(2\alpha T_c)^2}\right) d\omega. \quad (3.24)$$

We now consider the extent of the two Gaussian terms. The two variances are proportional to $\Delta\omega_s^2$ and $(2\alpha T_c)^2$. For our system $\Delta\lambda_s = 0.2 \text{ \AA}$ giving $\Delta\omega_s = 5.9 \times 10^{10} \text{ rad.s}^{-1}$, and $2\alpha T_c$ is simply equal to the laser frequency bandwidth. For our laser $\Delta\lambda = 8 \text{ nm}$ giving $\Delta\omega_{\text{laser}} = 2.36 \times 10^{13} \text{ rad.s}^{-1}$. Consequently, to an approximation, the second exponential term can be seen as limiting the temporal extent of the THz signal to approximately the width of the chirped pulse. This is an obvious and important physical restriction.

A number of inherent limitations of the chirped technique are highlighted by this analysis:

1. The temporal resolution is given by Eq. (3.22), and input THz pulses shorter than this will be distorted. Fletcher (2002) characterised the distortion and showed that it is dependent upon the modulation depth. This distortion causes ambiguities since similar output waveforms can result from dissimilar inputs.
2. The recovered THz spectrum is also distorted, in particular, high frequency components of the recovered spectrum are strongly attenuated.
3. Finally, only THz pulses that arrive during the window generated by the chirped probe pulse are detected. This limits the thickness variation of objects that are to be imaged without requiring the mechanical delay stage to be altered.

Figure 3.20 shows the THz signal measured using normal scanned electro-optic sampling and the chirped sampling method with a chirped pulse width of 21 ps. It is obvious that the THz pulse measured using the chirped probe pulse technique is significantly broadened. This broadening demonstrates the reduced temporal resolution and reduced frequency bandwidth of the chirped measurement technique compared with normal time scanned THz detection.

Hardware Setup

The hardware schematic for the chirped probe T-ray imaging system is illustrated in Fig. 3.21. The regeneratively amplified Ti:sapphire laser (Spectra Physics Hurricane)

3.3 Pulsed THz Imaging Architectures

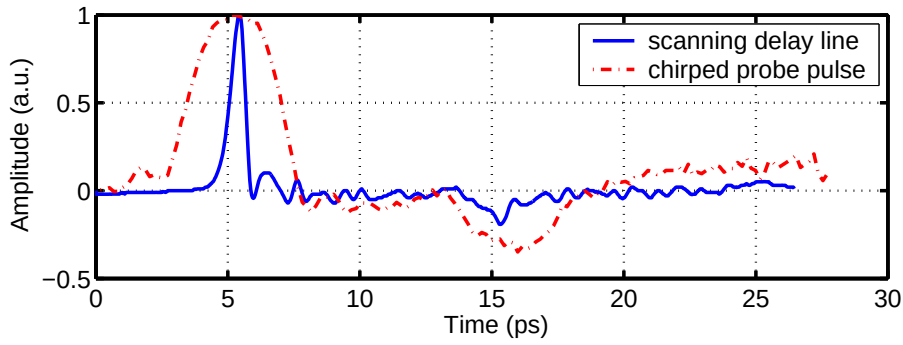


Figure 3.20. THz pulses measured with scanned EO sampling and EO sampling with a chirped probe pulse. The chirped pulse duration was 21 ps. This demonstrates the severe reduction in temporal resolution resulting from the chirped sampling technique.

described previously is used. The centre wavelength of the laser is 802 nm and the spectral bandwidth is 4 nm. The laser output is attenuated and split into pump and probe beams with powers of 30 mW and 20 μ W respectively. The terahertz emitter is a GaAs photoconductive antenna. A bias of 2 kV was applied to the emitter electrodes, which were spaced 16 mm apart. The average emitter current was approximately 100 μ A. This system generated an average THz power of approximately 5 μ W (5 nJ per pulse). The THz beam is focused using parabolic mirrors to a spot size of 2 mm at the sample. The transmitted THz pulse is collected using parabolic mirrors and focused onto the 4 mm thick $\langle 110 \rangle$ ZnTe EO detector crystal.

The optical probe pulse is linearly chirped using the grating pair. The grating pair (grating constant 10 μ m) is setup so that the grating separation is 4 mm and the angle of incidence is 51° , giving a chirped probe pulse width of 21 ps.

The chirped optical probe pulse and the terahertz pulse co-propagate in the ZnTe crystal. During this time the polarisation of the wavelength components of the optical pulse are modulated differently, depending on the temporal profile of the THz pulse. Crossed polarisers are used to convert this polarisation modulation to an amplitude modulation. The crossed polarisers ensure that the detected signal is approximately zero when no THz signal is present to prevent saturation of the CCD detector as discussed in Sec. 3.3.2. The background is not exactly zero due to residual birefringence in ZnTe, but this background is subtracted during processing, as specified in Eq. (3.18).

The temporal THz pulse is recovered by detecting the spectrum of the modulated pulse using a spectrometer grating (SPEX 500M) and the digital CCD camera (PI Pentamax) described in Sec. 3.3.2. Synchronised dynamic subtraction (see Sec. 3.3.2) is used to

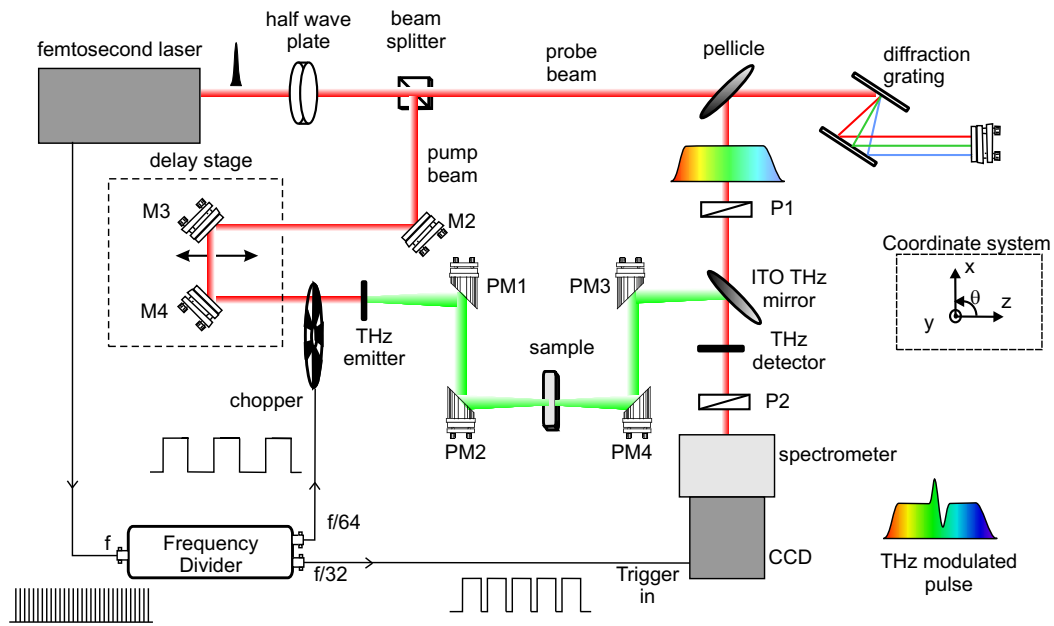


Figure 3.21. Schematic for chirped probe terahertz imaging. The probe beam is chirped using a diffraction grating to extend its pulse width from 130 fs to 21 ps. The pump beam generates THz pulses via a PCA emitter. The THz pulses are focused on the sample using parabolic mirrors PM1 and PM2, the transmitted radiation is then focused on the detector using PM3 and PM4. The THz pulse is reflected by an ITO beamsplitting mirror, which allows the chirped probe pulse and the THz pulse to propagate colinearly through the ZnTe detector. The wavelength components of the probe beam are then dispersed by a spectrometer and viewed on a CCD camera, revealing the THz temporal profile. The target is then raster scanned to acquire an image.

improve the CCD SNR. Using a CCD exposure time of 15 ms the SNR for the system was approximately 180. The CCD readout time was approximately 15 ms and the frame rate was set to 1/32 of the 1 kHz laser repetition rate, or approximately 32 fps. The sample is mounted on a X-Y translation stage and raster scanned to acquire an image.

Example Images

The chirped pulse technique is not without its drawbacks, and the reduction in temporal resolution has been noted by other authors (Sun et al. 1998, Riordan et al. 1998). This section presents spectra obtained using the chirped pulse method and discusses the limitations imposed in the time domain.

3.3 Pulsed THz Imaging Architectures

A number of samples consisting of different biological tissues were imaged using the chirped probe imaging system. An emphasis was placed on biological tissue as biomedical imaging is an important potential application of this technology.

The dried butterfly shown in Fig. 3.22 was imaged. The sample was scanned using the chirped probe THz imaging system with a scanning step size of $500\ \mu\text{m}$ and a total range of $7\ \text{cm} \times 7\ \text{cm}$. At each point the terahertz response was measured on the CCD using an exposure time of 15 ms. The entire image was acquired in 20 minutes. To demonstrate the richness of the data obtained using this technique a number of images are presented in Fig. 3.23. In Fig. 3.23(a) the peak amplitude of the THz pulse at each pixel is mapped to the grey scale intensity, for Fig. 3.23(b) each of the THz pulses is Fourier transformed to reveal the frequency domain information and the intensity of the spectra at a frequency of 0.2 THz is used as the grey scale intensity. Figure 3.23(c) shows the phase information in the THz pulses by measuring their delay at each pixel and then mapping this delay to the image intensity. Each of these three techniques yields different information about the sample under test and the optimal technique depends on the desired application. These three images can be combined, for example, by mapping each to a different colour (red, green or blue) axis to produce a pseudo-colour image that may have biomedical diagnostic value; an example of which is shown in Fig. 3.23(d).



Figure 3.22. An optical image of the pressed butterfly sample.

It is somewhat problematic to attempt to define a measure of image quality for THz imaging systems. A useful study was conducted by Fitzgerald et al. (2002). There are two major sources of noise in the images. The first is caused by the long term laser

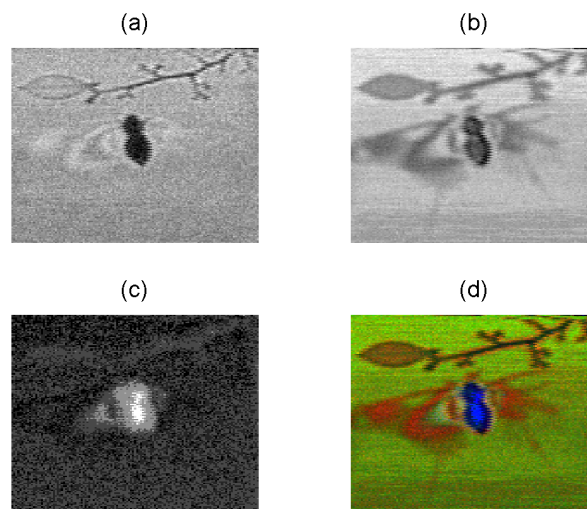


Figure 3.23. THz images of the pressed butterfly sample. The butterfly was imaged using the chirped THz imaging technique. The target was scanned in x (7 cm) and y (7 cm) dimensions with a resolution of $500\ \mu\text{m}$ and the THz response measured at each point. Image (a) was produced using the peak amplitude of the THz pulse at each pixel, image (b) was produced using by taking the Fourier transform of the THz response and using the amplitude at 0.2 THz for each pixel. Image (c) was produced by measuring the phase of the THz signal at each pixel. Image (d) was produced by combining (a), (b), and (c) on different pseudo-colour coded axes.

drift ($1/f$) noise in both the pump and probe beams. The second is shot noise in the CCD detector, which is proportional to the incident light intensity. These factors may be quantified in terms of the SNR of the measured THz field if no image target is inserted in the system. However, image quality is more difficult to define, as the visually observed image quality is largely dependent on the ratio of the contrast of the imaging target to the noise and will vary from target to target. A simple comparison of Figs. 3.23 and 3.24 illustrates this point. The leaf photographed in Fig. 3.24(a) was imaged using the chirped probe imaging system with exactly the same image parameters as Fig. 3.23, however the image quality is noticeably poorer. This is because the leaf absorbs much less of the incident THz radiation than the butterfly and therefore the image has poorer contrast.

Electro-Optic (EO) sampling with a chirped probe pulse results in a reduction in temporal resolution as discussed in Sec. 3.3.3, however it still offers extremely accurate phase measurements with a range resolution an order smaller than the wavelength

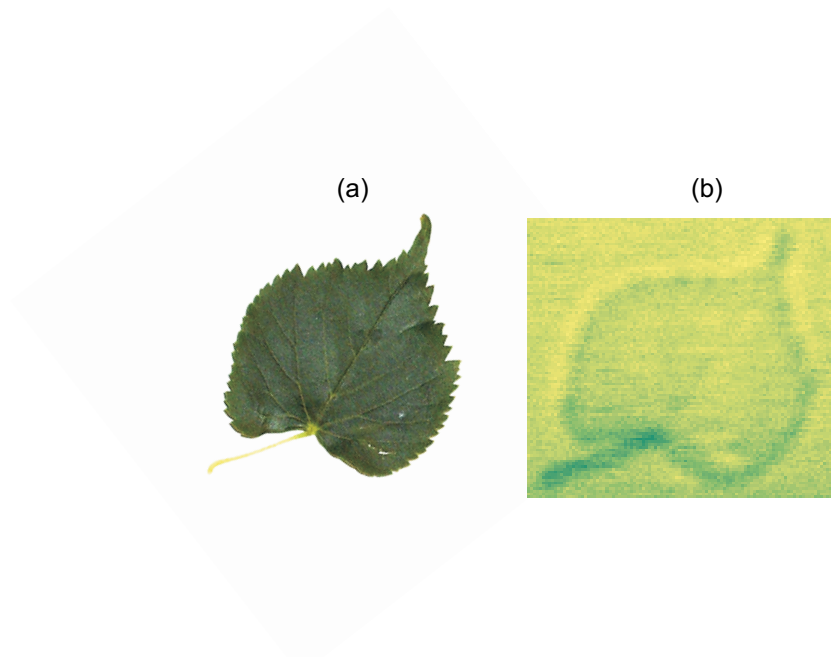


Figure 3.24. THz and optical images of a leaf. (a) Optical image of a leaf. The leaf was dried at ambient temperature for 12 hours before imaging. As a result the leaf has a reasonably low moisture content and therefore absorbs very little of the THz radiation. (b) A THz image of the leaf. The leaf was imaged using the chirped probe pulse THz imaging system and scanned with a spatial step size of 1 mm. The image acquisition took 15 minutes. The image was generated by plotting the THz amplitude at 0.2 THz at each pixel.

of the radiation. Figure 3.25 demonstrates the high temporal resolution of THz spectroscopy by plotting the measured THz pulses after transmission through different numbers of paper sheets. The paper used was 75 gsm flat white paper with a thickness (Δx) of $97\ \mu\text{m}$ and a dispersionless THz refractive index (n) of 1.88 over the frequency range 0.1 THz–3 THz. A single sheet of paper results in a delay of the THz pulse by $(n - 1) \times \Delta x / c = 285\ \text{fs}$, where c is the speed of light in a vacuum. Figure 3.25 shows the THz signal measured after transmission through different numbers of pages ranging from 1 up to 20. Figure 3.26 shows an enlargement of the peak of the THz pulse for the 1 and 2 page responses and clearly demonstrates that the 285 fs phase difference is distinguishable.

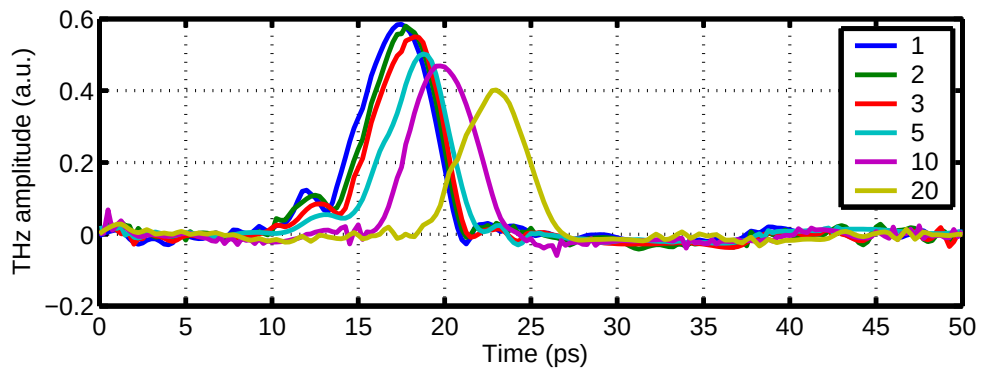


Figure 3.25. Terahertz responses of different numbers of pieces of paper. The chirped probe method results in reduced temporal resolution, but it is sufficient to detect the phase difference caused by a single piece of paper.

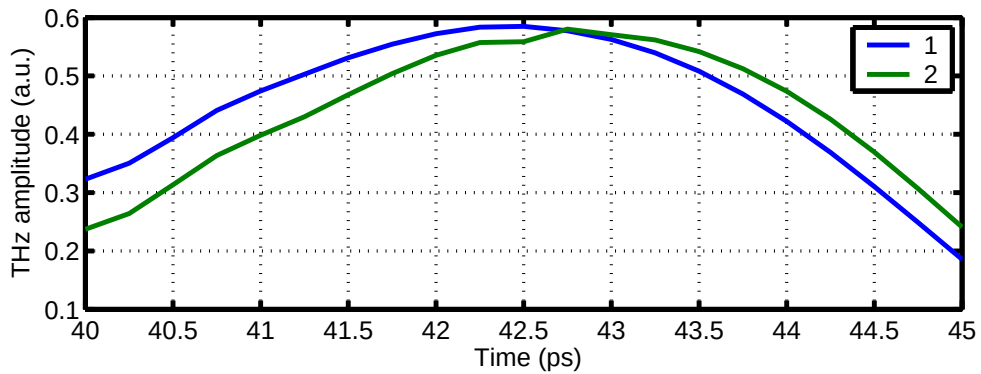


Figure 3.26. Zoomed view of THz responses of different numbers of pieces of paper. This plot highlights the peak of the THz pulses after transmission through 1 and 2 pieces of paper.

3.3.4 Other THz Imaging Methods

The three imaging systems identified in the previous sections are by no means the only available techniques. Several authors have suggested the construction of an array of photoconductive antennas for 2D detection of the spatial THz field (Hu and Nuss 1995); progress has been demonstrated on this front by Herrmann et al. (2002a) who demonstrated an 8 element PCA detector array. Quasi-optical THz imaging has been demonstrated (O'Hara and Grischkowsky 2001) along with a synthetic phased array method shown to improve the spatial resolution (O'Hara and Grischkowsky 2002, O'Hara and Grischkowsky 2004).

Other pulsed THz imaging systems with significant potential applications include impulse ranging for scale model radar cross section imaging (Cheville et al. 1997), and dark-field imaging (Löffler et al. 2001) for biomedical applications and industrial surface inspection. Progress is also being made using continuous wave THz sources. An imaging system using a THz quantum cascade laser has been demonstrated in imaging a rat brain histology sample, with a dynamic range of 1000 (Darmo et al. 2004). Incoherent THz radiation may be used for imaging through the technique of radio interferometry (Federici et al. 2003).

3.4 Chapter Summary

This Chapter has reviewed recent progress in the field of pulsed THz imaging and discussed its current advantages and disadvantages. It has presented in detail the three imaging techniques that form a basis for much of the research conducted in this Thesis. Several innovations were developed to increase the SNR of these techniques.

Traditional scanned THz imaging, based on THz-TDS, represents the most established and probably the most commonly used THz imaging technique due to its high SNR and simple setup. The need to raster scan the target and scan the delay stage results in long acquisition times but this may be improved using galvanometric delay stages and/or DSP acquisition.

THz imaging using 2D FSEOS offers many potential benefits over scanned imaging. The need to raster scan the target is removed and near real-time THz imaging is feasible. However, this method distributes the available THz power over all pixels and removes the LIA and therefore results in a significant reduction in SNR. Additionally the inhomogeneities inherent in large ZnTe crystals result in distortion of the THz image. Synchronised dynamic subtraction and sensor calibration techniques were developed to alleviate these disadvantages.

Terahertz imaging using a chirped probe pulse represents a recent addition to the available THz imaging techniques and promises to allow THz imaging and spectroscopy to extend to new applications in the monitoring of ultrafast phenomena due to its capacity for single shot measurements. The first ever transmission mode images measured using this technique have been presented.

The chirped imaging technique allows the full THz response of a single pixel to be measured simultaneously. This has advantages over other THz imaging techniques in

that if the sample moves during a scan the signature responses of the pixels are not corrupted, only the pixel to pixel intensity may change. Thus identification schemes such as those described in Ch. 5 should still succeed in classifying each pixel. However the chirped imaging technique does suffer from a number of disadvantages. The measured response is not linearly dependent on the THz pulse as indicated in Sec. 3.3.3, there is a limited temporal window over which the THz pulse may be detected. The SNR is also significantly lower than in time-scanning techniques.

With this foundation of THz imaging technologies, we are now in a position to develop the three dimensional (3D) tomographic imaging systems that form the focus of the next Chapter.

Chapter 4

Three dimensional THz Imaging

IN recent years T-ray imaging systems have advanced to a stage where practical applications are feasible. With this advance has come renewed interest in three dimensional imaging. T-ray tomography was first demonstrated in 1996 using reflected THz pulses in a B-scan ultrasound-like modality. However this method suffers from a number of limitations including the absence of spectroscopic information. This Chapter presents several novel T-ray tomographic methods based on *transmission* mode tomography. The hardware systems are described and mathematical approximations to the wave equation are derived to yield linear reconstruction algorithms that are capable of reconstructing a range of target materials.

Each of these techniques uses pulses of broadband THz radiation to obtain three dimensional images of targets with wide potential application. Images are presented demonstrating the performance of each technique along with a discussion of their relative advantages.

4.1 Introduction

“One cannot escape the feeling that these mathematical formulas have an independent existence and an intelligence of their own, that they are wiser than we are, wiser even than their discoverers, that we get more out of them than was originally put into them.”

- Heinrich Hertz (Bell 1937)

4.1 Introduction

The word tomography is derived from the Greek word *tomos* meaning ‘slice’ or ‘section’ and *graphia* meaning ‘describing’. The field of tomography involves methods for obtaining cross sectional images of a target, allowing the internal detail to be observed.

There is considerable interest in tomographic methods of THz imaging (Mittleman et al. 1997, Wang and Zhang 2002, Dorney et al. 2001b). These methods extend the advantages of 2-dimensional T-ray imaging (Hu and Nuss 1995) to applications involving 3-dimensional (3D) targets. Short pulses of broadband THz radiation are used to illuminate the target. Coherent detection methods are used to allow the reflected or transmitted THz pulse profile to be measured. This provides spectral information over a broad range in the important far-infrared band. In spectroscopy applications this information has been used for semiconductor characterisation (van Exter and Grischkowsky 1990c), the identification of gas mixtures (Jacobsen et al. 1996) and label-free DNA analysis (Nagel et al. 2002). A further advantage of this frequency range is the fact that many common materials including cloth, paper, plastics and cardboard are relatively non-absorbing. T-ray tomography systems therefore have a large number of potential applications.

Three novel techniques for transmission mode tomography using THz radiation are developed and demonstrated in this Chapter. After reviewing the current state of the art in tomographic imaging in the THz and neighbouring frequency bands, this Chapter will describe these methods in detail and discuss the applicability of each. These techniques are termed: T-ray Holography (Sec. 4.4), T-ray Diffraction Tomography (Sec. 4.5) and T-ray Computed Tomography (Sec. 4.6).

4.2 Review of Tomography Techniques

Techniques and reconstruction algorithms for tomographic imaging have been an active research topic for over a century. This field encompasses a wide range of disciplines and as such there is a rich body of background knowledge from which we are able to draw potential methods and algorithms for application in the THz band. In this section some of the most significant tomographic techniques are briefly reviewed to set the scene for analysis of T-ray tomographic methods. The review traverses the fields of X-ray CT, radio frequency (RF) tomography, 3D ultrasonic imaging as well as photonic imaging methods. Consequently, it does not attempt to provide a comprehensive review, choosing instead to highlight the most successful and innovative methods in each field.

4.2.1 X-ray Tomography

The most widely used algorithm for X-ray CT reconstruction is the filtered backprojection (FBP) algorithm, which was originally developed in an astrophysical setting (Bracewell and Riddle 1967). This algorithm provides excellent noise robustness, and may be implemented very efficiently. It is discussed in detail in Sec. 4.6.2. The filtered backprojection algorithm assumes that the measured signal is a line integral of the absorption coefficient of the target along the straight line between the source and detector. In practice this is only approximately true and as a result a number of alternative algorithms have been developed to reduce image artifacts that arise from practical non-idealities.

Beam-hardening artifacts are caused because the lower frequency components of a polychromatic X-ray beam are preferentially absorbed. This results in an increase in the mean energy of the beam as it propagates through the target, and therefore decreased attenuation. Thus the linear propagation model is no longer valid. If this effect is neglected the reconstructed image exhibit artifacts known as cupping, streaks and flares (Brooks and Di Chiro 1976, Duerinckx and Macovski 1978, Rao and Alfidi 1981, De Man et al. 1999). As a result polychromatic X-ray propagation models have been developed incorporating beam-hardening effects. Maximum Likelihood (ML) methods³ have greater flexibility for reconstructing X-ray images given more general

³Maximum likelihood methods (Fisher 1922) were developed by R. A. Fisher, who was a professor of The University of Adelaide 1959–1962. He died in Adelaide in 1962.

4.2 Review of Tomography Techniques

propagation models. The ML algorithm maximises the log-likelihood

$$L = \sum_{i=1}^I [y_i \cdot \ln(y_i - \hat{y}_i)], \quad (4.1)$$

where $\{y_i\}_{i=1}^I$ is the set of transmission measurements, $\hat{y}_i$ is the expected measurement along the given projection line i for the current reconstructed image and propagation model. Here, y_i is assumed to be a Poisson realisation of $\hat{y}_i$.

The reconstructed image is then iteratively updated to maximise L . A number of methods have been developed to update the estimate of the reconstructed image (Lange and Carson 1984, Fessler et al. 1997). De Man et al. (1999) demonstrated an iterative maximum-likelihood polychromatic algorithm for CT (IMPACT), incorporating energy dependent absorption and energy dependent Compton scattering that exhibited a marked improvement over the FBP algorithm for their simulations.

Similarly, expectation maximisation (EM) algorithms are used to reconstruct the data from modern cone beam CT scanners, which provide higher spatial resolution and faster image acquisition than parallel ray CT imagers (Manglos et al. 1995, Nuyts et al. 1998).

4.2.2 Optical Tomography

Optical tomography refers to the use of optical or NIR radiation to probe highly scattering media, most commonly in association with human tissue. A wide range of experimental techniques exist using both CW illumination and pulsed illumination with time domain detection. The Boltzmann equation governs photon transport in scattering media. In the time domain it is given by

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \hat{\mathbf{s}} \cdot \nabla + \mu_{\text{tr}}(\mathbf{r}) \right) \phi(\mathbf{r}, \hat{\mathbf{s}}, t) = \mu_s(\mathbf{r}) \int_S \Theta(\hat{\mathbf{s}}, \hat{\mathbf{s}}') \phi(\mathbf{r}, \hat{\mathbf{s}}', t) d\hat{\mathbf{s}}' + q(\mathbf{r}, \hat{\mathbf{s}}, t), \quad (4.2)$$

where $\phi(\mathbf{r}, \hat{\mathbf{s}}, t)$ is the number of photons per unit volume at position $\mathbf{r}$ at time t with velocity in direction $\hat{\mathbf{s}}$, $\mu_s(\mathbf{r})$ is the scattering cross-section at position $\mathbf{r}$, with units of photons per metre, μ_a is the absorption cross section and $\mu_{\text{tr}} = \mu_s + \mu_a$ is the transport cross-section. Here, $\Theta(\hat{\mathbf{s}}, \hat{\mathbf{s}}')$ is the normalised phase function representing the probability of scattering from direction $\hat{\mathbf{s}}$ to direction $\hat{\mathbf{s}}'$, $q(\mathbf{r}, \hat{\mathbf{s}}, t)$ is the source term, which is assumed to be isotropic and has units of photons per metre, and S is the unit sphere.

The *diffusion approximation* simplifies the Boltzmann equation by defining the photon density $\Phi(\mathbf{r}, t) = \int_S \phi(\mathbf{r}, \hat{\mathbf{s}}, t) d\hat{\mathbf{s}}$ and photon current $J(\mathbf{r}, t) = \int_S \hat{\mathbf{s}} \phi(\mathbf{r}, \hat{\mathbf{s}}, t) d\hat{\mathbf{s}}$, each with units of photons per unit volume. The reduced scattering coefficient $\mu'_s = (1 - g)\mu_s$ and the diffusion coefficient, $\kappa = \frac{1}{3(\mu_a + \mu_s)}$ are also defined where g is the dimensionless scattering anisotropy. The diffusion approximation assumes that $\frac{\partial J}{\partial t} = 0$, yielding (Arridge 1999)

$$-\nabla \cdot \kappa(\mathbf{r}) \nabla \Phi(\mathbf{r}, t) + \mu_a \Phi(\mathbf{r}, t) + \frac{1}{c} \frac{\partial \Phi(\mathbf{r}, t)}{\partial t} = q(\mathbf{r}, t). \quad (4.3)$$

Repeated measurements are conducted using multiple source and detector locations in either a transmission or reflective geometry. Most common reconstruction algorithms use iterative methods to invert the diffusion equation using numerical inversion techniques. In these methods a recursive finite element model is used to solve the forward problem and a solution is determined iteratively using methods such as the Levenberg-Marguardt algorithm (Singer et al. 1990, Paulsen and Jiang 1995, Oleary et al. 1995, Gao et al. 2000). These methods show promise, however there is no guarantee of convergence and they are computationally expensive, especially in 3D. A wide range of alternative techniques have been developed. By Fourier transforming Eq. (4.3) a backpropagation operator may be defined to allow the photon density on a plane perpendicular to the photon propagation direction to be reconstructed (Matson et al. 1997, Matson and Liu 1999), this method has been demonstrated experimentally for breast phantom imaging (Liu et al. 1999).

A number of authors have sought to simplify the diffusion relation to one that is amenable to simple backprojection operators such as those used for X-ray reconstruction. These methods often employ the approximation of a macroscopically homogeneous medium (Feng et al. 1995, Walker et al. 1997) and result in only qualitative reconstructed images. Using time gated detection techniques and a short pulse excitation, the ballistic component of the transmitted light can be isolated from the scattered component (Yoo et al. 1991). Linear algorithms may then be applied with higher accuracy (Chen and Zhu 2001). This technique may be improved by adding a deconvolution stage to the backprojection algorithm to correct for the point spread function of the scattering media (Colak et al. 1997).

4.2.3 RF Tomography

The propagation of electromagnetic radiation is governed by Maxwell's equations. In most cases at microwave frequencies these equations reduce to the Helmholtz equation, which forms the basis for both microwave and ultrasound tomography. These methods are commonly referred to as diffraction tomography.

Inverse electromagnetic problems have application in subsurface imaging for mining exploration and biomedical imaging. Researchers have typically followed one of two paths. The first involves making linear approximations to the Helmholtz equation and directly inverting the resulting relation (Wolf 1969, Devaney 1982). This method was adopted to reconstruct THz images of targets and a detailed derivation of these techniques is presented in Sec. 4.5. The second, more arduous option attempts to invert the nonlinear Helmholtz equation using iterative methods (Borup et al. 1992, Gutman and Klibanov 1993).

Most of the iterative methods define a forward model for the wave equation. This forward model is used to simulate the scattered field that would be observed at the receivers based on the current estimate of the target's object function. The error between the actual measured field and the simulated field is used as an objective function and is minimised by iterative numeric techniques. Forward modelling of the full-wave electromagnetic problems is an extremely computationally intensive task and is typically addressed using finite element models (Druskin and Knizhnerman 1994, Murch et al. 1988). For reasonable sized 3D problems this method is not feasible on current computing technology and much research is focused on improving the efficiency by improved computational techniques, (Paulsen et al. 1996), by using simpler forward models such as the Distorted Born Approximation (Habashy et al. 1993, Wombell and Murch 1993), or by reconstructing only the shape of the target (van den Berg et al. 1995).

Recently a number of iterative techniques have been developed that avoid the requirement of implementing a forward solver at each iteration. Principle among these algorithms are the modified gradient in field (MGF) method and the contrast source inversion (CSI) technique. Both of these methods minimise a scalar cost function using iterative conjugate gradient optimisation schemes. In MGF the unknown variables are the total field and the material contrast at each position on the reconstruction grid. The cost function is the sum of the errors in the measured data and a domain integral equation (Kleinman and van der Berg 1992, Kleinman and van der Berg 1994). While

for CSI a quantity referred to as the *contrast source*, w_i , is defined as the product of the total field and the material object function at each grid position. Numerical methods are then used to iteratively determine the contrast source, the total field and the object function at each grid position (van den Berg and Kleinman 1997, van den Berg 1999, Abubakar and van den Berg 2002).

4.2.4 Ultrasound Tomography

Reflection mode ultrasound systems are ubiquitous and offer high contrast images in a range of applications. Transmission mode ultrasound tomography is a more demanding problem. The hardware is more involved and must include emitters and detectors surrounding the target. A prototype system has been developed by Jansson et al. (1998). Ultrasound propagation can be described by the Helmholtz equation so many of the methods employed for electromagnetic tomography may be applied to ultrasound tomography (Natterer and Wübbeling 2001, Devaney 1982). The state of the art (albiet computationally expensive) is the propagation-backpropagation (PBP) algorithm of Natterer and Wübbeling (1995).

4.3 Review of THz Tomography Techniques

In recent years a number of methods for 3D imaging with THz radiation have been proposed and demonstrated. Even prior to the development of pulsed THz systems, gas laser CW THz sources were used for 3D imaging and radar cross-section (RCS) measurements of scale models of military aircraft (Waldman et al. 1979). Since the development of pulsed THz systems, such 3D imaging systems have flourished. Traditional reflection mode THz tomography techniques were reviewed in Sec. 1.3.

The following sections provide a relatively detailed review of several recent techniques that have particular relevance to the tomographic methods proposed and demonstrated in this Thesis. This field is also reviewed in Wang et al. (2004) and Wang et al. (2003a).

4.3.1 Tomography with a Fresnel Lens

Diffraction Fresnel zone plates, or Fresnel lenses may be used to focus light in place of traditional refractive lenses (Jahns and Walker 1990). Fresnel lenses often have size

4.3 Review of THz Tomography Techniques

and weight advantages over refractive lenses, however they are generally favoured for narrowband applications due to their frequency dependent focal length. Wang and Zhang (2002) demonstrated that this frequency-dependence may be utilised to perform tomographic THz imaging. A Fresnel lens is constructed by machining a dielectric material in a series of concentric circles with varying depth as illustrated in Fig. 4.1.

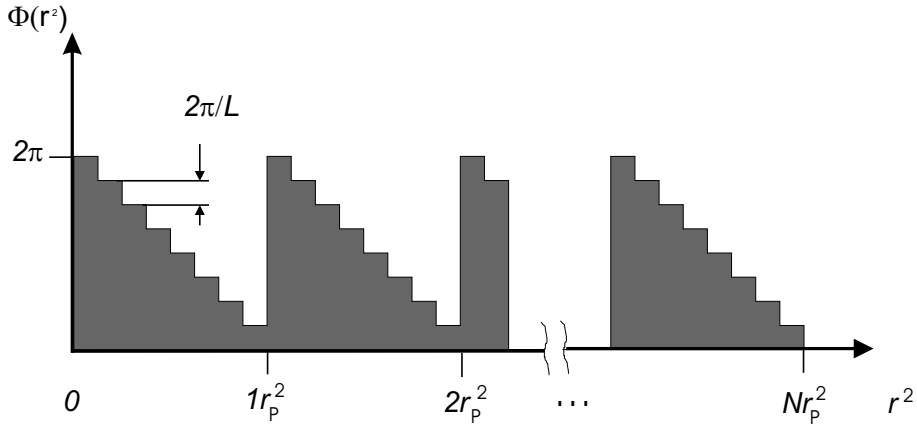


Figure 4.1. Profile of a multi-level Fresnel zone plate. The lens is constructed by patterning an array of concentric circles at different depths. The graph shows the phase change, $\phi(r^2)$, imparted by the lens as a function of radius squared, r^2 . Here, L is the level number of the lens and N is the number of zones. After (Wang et al. 2002b, Walsby et al. 2002b).

The focal length of a Fresnel lens is given by (Jahns and Walker 1990)

$$f_\nu = \frac{r_p^2}{2\lambda} = \frac{r_p^2}{2c} \nu \propto \nu, \quad (4.4)$$

where r_p^2 is the Fresnel zone period with a dimension of area, λ is the wavelength, and c is the speed of light. The focal length f_ν of a Fresnel lens is linearly proportional to frequency ν . This unique property allows tomographic imaging of a target when used with broadband illumination (Ferguson et al. 2002d, Wang et al. 2002a, Walsby et al. 2002a). Using a Fresnel lens, and considering the image formed by radiation at each different frequency, it is possible to image the objects at various positions along the beam propagation path onto a fixed imaging plane. This procedure enables the reconstruction of an object's 3D tomographic contrast image.

For a single-lens imaging system, under the paraxial ray approximation, the thin lens equation,

$$\frac{1}{z} + \frac{1}{z'} = \frac{1}{f_\nu}, \quad (4.5)$$

relates the object distance z , the image distance z' and the focal length f_ν of the lens. The magnification of the image is given by $(-z'/z)$. In an imaging system the image plane position, z' , is fixed. Since the lens focal length is frequency dependent, the object distance z is also a function of frequency. Combining Eq. (4.4) and Eq. (4.5) yields,

$$z = \frac{f_\nu z'}{z' - f_\nu} = \frac{r_p^2 z' \nu}{2cz' - r_p^2 \nu}. \quad (4.6)$$

Therefore at each illumination frequency, the image formed at z' corresponds to a focused image of a plane through the target at a different depth, z . Obviously to obtain real (non-virtual) images requires $z > 0$ and hence $z' - f_\nu > 0$, implying that $\nu < 2cz'/r_p^2$.

This tomography system has been demonstrated for imaging simple targets consisting of different shapes cut from polyethylene sheets. The experimental setup was similar to the 2D FSEOS system detailed in Sec. 3.3.2. A 30 mm diameter silicon binary lens with a focal length of 2.5 cm at 1 THz was used as the THz wave Fresnel lens. By scanning the time delay between the THz and optical probe beams, a temporal waveform of the THz wave at each pixel on the image plane was measured using a CCD camera. Fourier transformation of the temporal waveforms provided the THz field amplitude (or intensity) distribution on the image plane at each frequency. The measured two-dimensional THz field distribution at each frequency formed an image of a target at a corresponding position along the z -axis.

Figure 4.2 schematically illustrates the tomographic imaging arrangement and experimental results. Three plastic sheets with different patterns were placed along the THz beam path, and their distances to the lens, corresponding to z in Eq. (4.6) were 3 cm, 7 cm and 14 cm, respectively. Inverted images of patterns on the sensor plane at distance $z' = 6$ cm were measured at frequencies of 0.74 THz, 1.24 THz, and 1.57 THz, respectively. At each frequency, the Fresnel lens imaged a different plane section of a target object corresponding to a certain depth, while images from other depths remained out of focus. Each point in the different object planes along the z -axis was mapped onto a corresponding point on the z' plane (sensor plane) with the magnification factor $-z'/z$ at their corresponding frequencies.

A Fresnel lens allows 3D tomographic images to be obtained from a single 2D THz image. Using a single projection image, the THz spectral data provides sufficient information to reconstruct the full 3D target. Although this method does not provide

4.3 Review of THz Tomography Techniques

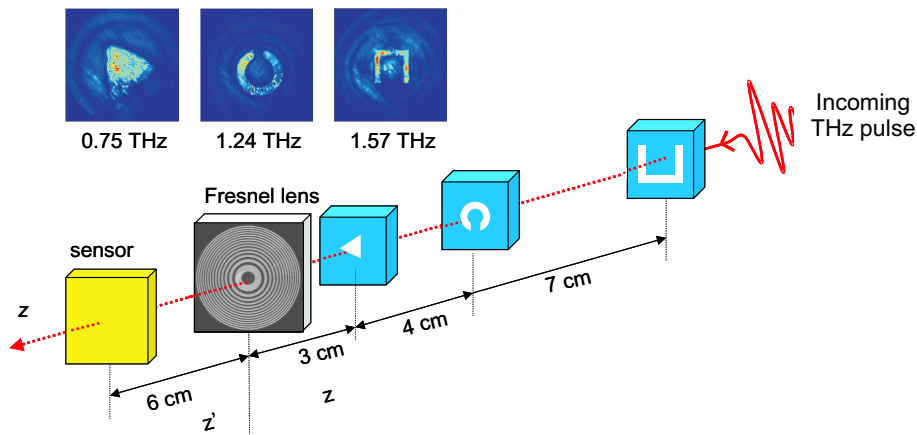


Figure 4.2. Schematic illustration of tomographic imaging with a Fresnel lens. Targets at various locations along the beam propagation path are uniquely imaged on the same imaging sensor plane with different frequencies of the imaging beam. Three plastic sheets were cut with different patterns placed 3 cm, 7 cm, and 14 cm away from the Fresnel lens. The patterns are imaged on the sensor at a distance of 6 cm from the Fresnel lens, with inverted images of the patterns forming at frequencies of 0.75 THz, 1.24 THz and 1.57 THz, respectively. The measured image size is determined by the frequency dependent magnification factor, defined as $-z'/z$. The images are inverted, both vertically and horizontally, as a result of the negative magnification factor. After (Ferguson et al. 2002d, Wang and Zhang 2002).

spectroscopic information it has the potential to acquire 3D images of targets extremely quickly.

The resolution of this technique in the z dimension is largely determined by the depth of focus of the THz wave. The depth uncertainty of the target position is equal to the depth of focus divided by the square of the magnification factor (Saleh and Teich 1991), the uncertainty of the target position is also a function of z . The measured depth of focus in the demonstrated system was 3 mm (Wang and Zhang 2002). For a large value of z ($z \gg z'$), the depth resolution decreases, which reduces the usefulness of this system for large targets or mid-range imaging. This concept has been demonstrated using a broadband THz radiation as the imaging beam, however it is also applicable to tunable narrowband imaging systems, and can be applied to other frequency ranges, including the visible and RF regimes (Minin and Minin 2000).

4.3.2 Time Reversal Imaging

Time reversal imaging is an innovative indirect imaging method demonstrated with pulsed THz radiation by Ruffin et al. (2001). By exploiting the time-reversal symmetry of Maxwell's wave equations they derived an image reconstruction algorithm based on the time-domain Huygens-Fresnel diffraction equation. This method allowed them to reconstruct 1D, 2D and 3D (Buma and Norris 2003) amplitude and phase contrast objects based on measurement of the diffracted THz field at multiple angles.

The diffraction of broadband electromagnetic pulses in free space is described by the time-domain Huygens-Fresnel diffraction formula

$$u(P_0, t) = \int \int_{\Sigma} \frac{\cos \theta}{2\pi c r_{01}} \frac{\partial}{\partial t} u \left(P_1, t - \frac{r_{01}}{c} \right) d\sigma, \quad (4.7)$$

where $u(r, t)$ is the electric field as a function of position and time, P_1 is a point on the object, P_0 is a point in the far-field on the measurement plane, r_{01} is the distance between the points, c is the speed of light and θ is the zenith angle made by the line joining P_0 and P_1 with the wave vector of the incident radiation. This equation allows the field on a distant plane to be calculated by integrating the time derivative of the field at the object plane $u(P_1, t - \frac{r_{01}}{c})$ over an aperture Σ , where $d\sigma$ is an infinitesimal aperture element.

Ruffin et al. (2001) demonstrated that the time symmetry of Eq. (4.7) can be exploited to allow the field at the object plane P_1 to be determined based on measurement of the diffracted field P_0 at several off-axis positions. This method makes use of the phase information inherent in THz-TDS measurements. For their target geometry, as shown in Fig. 4.3, the reconstruction algorithm for the field at the target plane was shown to be

$$u(P_1, t) = -\frac{1}{4\pi c} \int \int_{\Sigma'} (1 + \cos \theta) \times \frac{\partial}{\partial t} u \left(P_0, t + \frac{r_{01}}{c} \right) d\sigma', \quad (4.8)$$

where $u(P_0, t + r_{01}/c)$ is the time reversed measured scattered field, and the integral is performed over the measurement sphere (or semicircle for 1D reconstructions).

This method was extended to allow 2D targets to be imaged by fixing the detector at a given zenith angle ($\theta \neq 0$), rotating the object about the optical axis (the axis of the wave vector) and measuring the diffracted field for multiple rotation angles. This allowed the diffracted field to be sampled on a hemisphere and Ruffin et al. (2002)

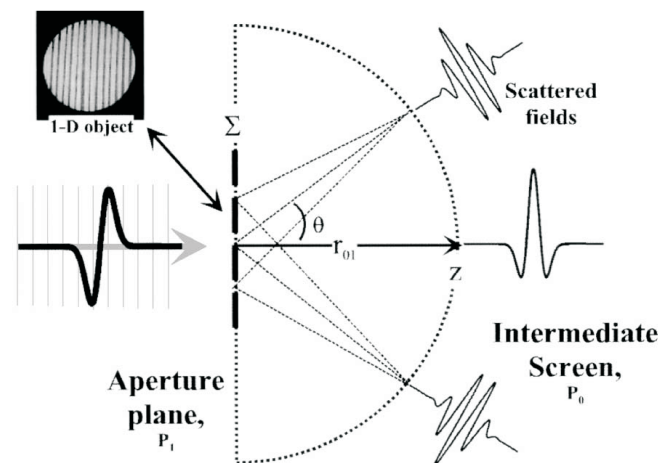


Figure 4.3. 1D time reversal imaging setup. A collimated THz beam was incident on a target, in this case a grating pattern. The scattered THz field was measured on a semicircle at a radius of r_{01} . In practice this was achieved by mounting a fibre coupled THz detector on a pivoting arm. After (Ruffin et al. 2001).

showed that the multiple frequencies present in the broadband THz radiation allow the spatial Fourier transform of the object to be sampled sufficiently to provide an accurate reconstruction. This 2D reconstruction was applied to a 10 mm diameter star pattern and the resultant reconstructed image is shown in Fig. 4.4. The top image in Fig. 4.4 shows a conventional scanned image of the star target. This image required the THz response to be measured at 8,100 pixels, while the time reversal image only required the THz response to be measured for 72 different rotation angles of the target. This represents a considerable saving in acquisition time and demonstrates the power of this technique.

The resolution of this method was derived using the Sparrow criterion (Sparrow 1916), which states that two peaks are resolved if there is a clear local minimum between the principal peaks of the two waveforms. This definition allowed the high temporal resolution of THz-TDS systems to be leveraged to derive the spatial resolution. The resolution is given by the spatial separation of two points on the object plane that give rise to THz pulses with an observable timing difference at the detector. Using this method a resolution of $674 \mu\text{m}$ was demonstrated, which was significantly smaller than the mean wavelength of the THz source used. Time reversal THz imaging was also demonstrated for phase contrast targets and for reflection mode imaging (Ruffin et al. 2002).

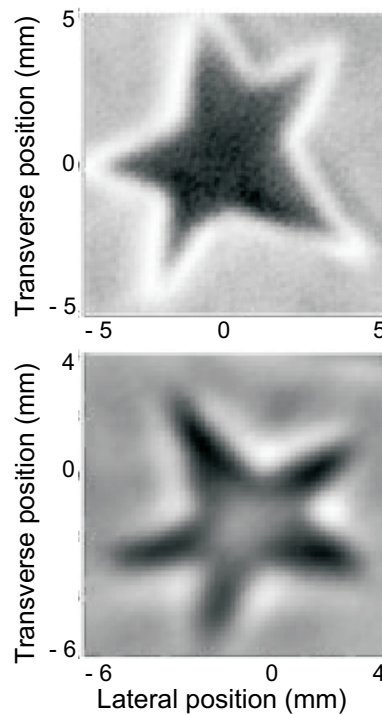


Figure 4.4. 2D time reversal image of a 10 mm wide star pattern. (Top) a conventional scanned THz image of a star pattern cut in a business card. (Bottom) Image formed by time reversal of the diffracted field measured for 72 different rotation angles of the target. The image quality is similar for each image, however, the conventional THz image required 8,100 measurements while the image on the bottom required only 72 measurements. After (Ruffin et al. 2002).

4.3.3 Multistatic Imaging

Time reversal imaging is one of a broad class of multistatic imaging techniques where multiple detectors are positioned to capture the scattered radiation at different angles. These methods are also termed indirect imaging methods as a reconstruction algorithm must be applied to recover the target image. In most cases a single THz detector is used and the measurement is repeated for different rotation angles of the target or different positions of the detector, however the principle is identical to multistatic imaging.

Kirchhoff Migration

Dorney et al. (2001b) utilised principles from geophysical prospecting to demonstrate THz reflection imaging using Kirchhoff migration. This method highlighted the potential of THz-TDS systems to provide a table-top testbed for 'seismic' imaging. The

4.3 Review of THz Tomography Techniques

measurement principle is illustrated in Fig. 4.5. An array of detectors is simulated by repeating the THz-TDS measurement as the detector is translated across the top of the measurement plane. An emitter, positioned on the same plane directs pulses of THz radiation at the target and the detector measures the time of arrival of the reflected pulse at each position.

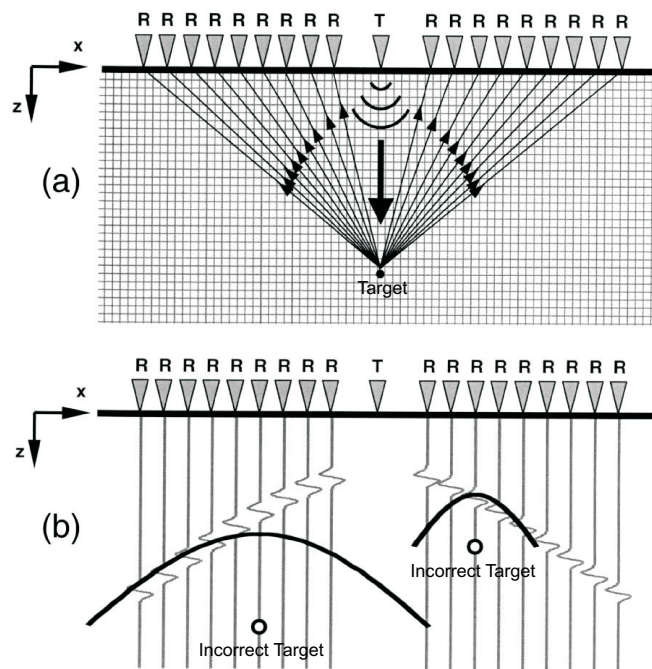


Figure 4.5. The measurement geometry used for Kirchhoff migration imaging. (a) A single transmitter (T) directs THz radiation in the z direction towards the target. An array of detectors (R) measure the reflected signal caused by the target. In practice this arrangement is simulated by translating a detector and repeating the measurement for each detector position. The travel time of the pulses recorded on a regularly spaced array of detectors form a hyperbola (indicated by the arrow heads). (b) The Kirchhoff migration algorithm iteratively assumes the position of the target on a reconstruction grid. The hyperbola that would result from a target at the given grid position is calculated and compared with the observed THz return along that hyperbola. The correlation is high when the grid position coincides with the target location and low otherwise. The hyperbola for two incorrect target positions are shown. After (Dorney et al. 2001b).

This method provides 2D (x, z) reconstructions of reflecting targets and conceptually is easily extended to 3D by measuring the reflected THz field on a square array at the 'surface'. Translating a single detector will result in prohibitive image acquisition times for 3D imaging, however a much faster system can be envisaged using the 2D FSEOS THz imaging system described in Sec. 3.3.2. One disadvantage of applying 2D FSEOS

to Kirchhoff migration is the fact that the fidelity of the target reconstruction is related to the span of the receiver array (Dorney et al. 2002). For the 2D FSEOS system, this span is limited by the size of the ZnTe detector. Large detector crystals are prohibitively expensive.

Seismic processing techniques have also been applied to allow not only the shape and position of targets to be imaged, but also to allow their refractive index to be estimated. This is a difficult problem as both the thickness and the refractive index (or equivalently the wave velocity) are unknown. Nevertheless Dorney et al. (2002) have demonstrated reconstruction of the refractive index of layered strata of Teflon and polyethylene using a semblance metric based on the quality of the reconstructions and iteratively guessing the refractive index of the layers (Neidell and Taner 1971, Dix 1955).

Synthetic Aperture Radar

An early application emphasis for THz systems was in performing radar cross-section (RCS) measurements of scale models of military vehicles and aircraft as an inexpensive alternative to operational trials (Waldman et al. 1979, Cheville and Grischkowsky 1995b, Cheville et al. 1997).

This concept has been extended through the demonstration of a small scale synthetic aperture radar (SAR) based on THz impulse ranging (McClatchey et al. 2001). In this system a 1:2,400 scale model of a destroyer class ship was imaged and the scattered radiation was measured for 20 different angles. The SAR reconstruction algorithm is not dissimilar to the time reversal algorithm employed in Sec. 4.3.2, however it is applied in the frequency domain. The target is considered to be a set of point scatterers. The phases of the measured Fourier coefficients for all angles are backpropagated to the target plane, where they constructively reinforce wherever a point scatterer exists (Soumekh 1999). The reconstructed THz image of the destroyer model is shown in Fig. 4.6. One notable aspect of THz impulse ranging is that while the lateral resolution is typically limited by the Rayleigh criterion to the order of the peak THz wavelength, the depth resolution is dependent on the spectral bandwidth of the THz pulses. For a typical pulse with a rise time of $\Delta t = 0.8$ ps the range resolution is $\Delta t/2 \times c = 0.12$ mm, which is almost an order of magnitude smaller than the peak wavelength.

4.4 T-ray Holography

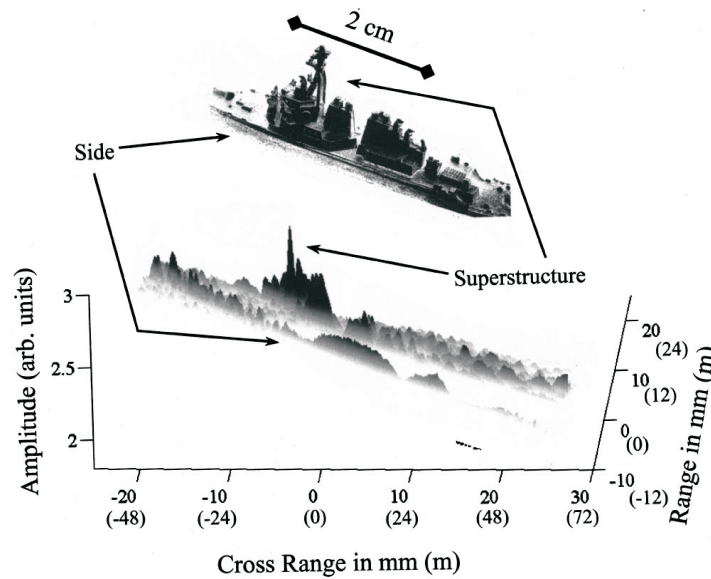


Figure 4.6. Scale model (1:2,400) of a destroyer imaged using THz SAR. (above) an optical photograph of the model (below) the model was illuminated with a 15 mm wide $(1/e)$ Gaussian THz wave and the scattered field was measured over a 20° angular range at 1° intervals. The measured signals were backpropagated to the target location and the result surface rendered. The superstructure and side of the model are reconstructed reasonably accurately. After (McClatchey et al. 2001).

4.4 T-ray Holography

4.4.1 Introduction

We now move on to discuss the first of three tomographic imaging techniques developed in this Thesis. 3D T-ray holography is a novel extension of recent work in THz imaging using time-reversal of the Fresnel-Kirchhoff equation (see Sec. 4.3.2). It allows 3D images of point scatterers to be obtained using 2D FSEOS THz imaging (see Sec. 3.3.2). The reconstruction algorithm is based on the windowed Fourier transform and allows extremely rapid 3D imaging (Wang et al. 2003b, Wang et al. 2004).

Digital holography records holograms using a CCD, and then employs computer algorithms to reconstruct the digitised holograms according to Fourier optics theory (Yamaguchi et al. 2001, Kim 1999). The rapid progress in computer and information

technology has made digital holography systems practical, and they have numerous applications in 3D imaging (Testorf and Fiddy 1999) and information security (Javidi and Nomura 2000) applications.

To generate holograms, both the intensity and the phase distribution must be recorded. In most common holographic technologies, the intensity and phase distribution are measured through recording an image of the interference pattern formed by the object and reference waves. THz-TDS provides coherent measurement of the THz electric field $E(t)$ as a function of time, rather than the intensity $|E(t)|^2$ (Mittleman et al. 1998b). As a result, the phase information is preserved and one can determine both the real and imaginary parts of the THz wave at each frequency via Fourier Transformation. This allows THz holograms to be directly recorded without the use of a reference wave. Eliminating the reference wave also leads to more reliable hologram.

In addition to the phase and amplitude information at each frequency, THz pulses also contain temporal information that may be used to reconstruct 3D holographic images. When THz pulses are scattered by multiple scattering centres, the peaks of the scattered pulses arrive at the detector at different time delays depending on the scattered wave propagation paths; these time delays can then be used to differentiate between pulses that propagated along different scattering paths. Thereby depth information concerning the scattering centres can be extracted.

The T-ray holography technique developed in this Thesis utilises the windowed Fourier transform in an algorithm for the reconstruction of 3D tomographic holograms, this method is most applicable for the identification of point scatterers in a homogenous background.

4.4.2 2D T-ray Holography

To demonstrate digital terahertz holography, the 2D FSEOS THz imaging system described in Sec. 3.3.2 is used. An OR THz emitter, consisting of a 3 mm thick $\langle 110 \rangle$ oriented ZnTe crystal, is used to provide a wide THz bandwidth and thereby improved spatial resolution.

The 2D FSEOS system allows the diffraction pattern caused by a target to be measured. Before considering 3D reconstruction of the target we investigate the reconstruction

4.4 T-ray Holography

of a 2D target profile. The reconstruction is based on time-reversal of the Huygens-Fresnel diffraction integral Eq. (4.7) using a method similar to that of Ruffin et al. (2001).

Previous implementations of this technique have all relied on a single THz detector, and have required the THz measurement to be repeated for several different detector positions to ensure that the diffracted field was collected over a wide enough angular range. In the case of Ruffin et al. (2001) this required the measurement of THz waveforms at 72 different detector positions to allow a 1 dimensional reconstruction; for a 2D reconstruction the target also had to be rotated and the measurements repeated. The method proposed here potentially allows a 2D reconstruction to be performed using only 1 measurement. This represents an acceleration of several orders of magnitude relative to previous methods and promises to allow near real-time implementation!

However, one disadvantage of this method over the single detector technique is that the angular range over which the diffracted radiation can be collected is necessarily reduced. This is due to the fact that the ZnTe detector cannot be placed arbitrarily close to the target, and ZnTe crystals cannot (cost effectively) be made arbitrarily large. The ZnTe crystal used in this experiment had a diameter of 20 mm and was placed 48 mm from the target, allowing the diffracted radiation to be collected over an angular range of $\pm 11^\circ$. An obvious solution to this problem is to simply rotate the target, however in this case the acquisition time becomes dramatically longer and, as it will be shown in Sec. 4.5 and Sec. 4.6, more powerful reconstruction techniques may then be used to provide additional information.

Young's Double Slit Experiment

A THz variation of the traditional Young's double slit experiment (Young 1804) was performed using the 2D FSEOS imaging system. The geometry of the experiment is shown in Fig. 4.7. Two vertical slits were cut in an aluminium foil mask. The slit width was 1 mm and the slit separation was 6 mm. The illuminating THz wave was coherent and polychromatic. The radiation is diffracted at the slits, which act as the source of secondary wavelets. The distance to the sensor D is much greater than the wavelength and hence can be considered to be in the far field, which is a requirement for the applicability of the Fresnel diffraction equation (Saleh and Teich 1991). The two waves interfere and form an interference pattern on the ZnTe sensor.

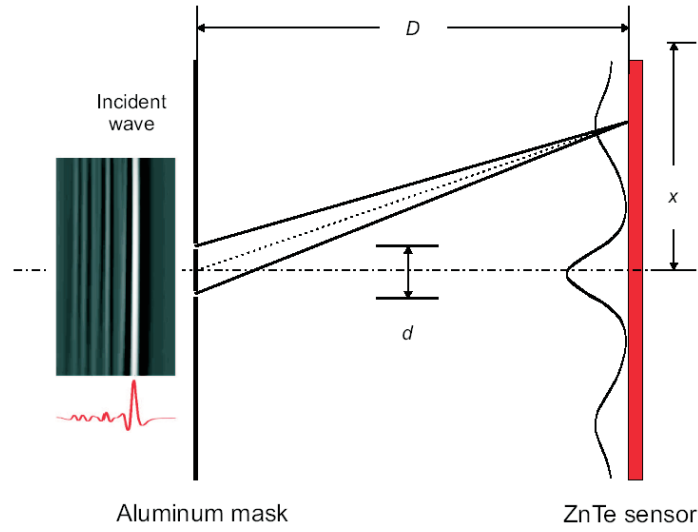


Figure 4.7. Schematic of Young's double slit experiment. The 2D FSEOS THz imaging system was used to perform the interference experiment. Two slits, with widths of 1 mm, and a separation (d) of 6 mm were patterned in an aluminium foil mask. The target was illuminated with a THz plane wave and the diffraction pattern measured on the ZnTe detector at a distance (D) of 48 mm. Note that the probe beam and ITO mirror shown in Fig. 3.16 are not shown for simplicity. After (Wang et al. 2004).

The time domain diffraction pattern is shown in Figs. 4.8 and 4.9. The circular wavelets formed by each of the slits are clearly visible as are their mutual interference effects. Traditionally Young's double slit experiment is performed using quasi-monochromatic light, which allows interference fringes to be observed. To show similar effects using the THz data the Fourier transform of the time domain data was obtained. This gives rise to interference images at each frequency. Figure 4.10 shows 4 such images at frequencies of 0.4 THz, 0.8 THz, 1.2 THz and 1.6 THz. For quasi-monochromatic light, the light intensity on the detector is a function of x and is given by

$$I(x) = 2I_0 \left[1 + V \cos \left(\frac{2\pi\theta}{\lambda} x + \phi \right) \right], \quad (4.9)$$

where λ is the wavelength of the radiation, I_0 is the incident light intensity, V and ϕ are measures of the amplitude and phase of the spatial coherence of the light at the two slits, and $\theta = d/D$. That is, the fringe separation is given by $D\lambda/d$. This relationship is illustrated in Fig. 4.10. The fringe separation was measured for each frequency diffraction image and the fringe separation plotted against wavelength in Fig. 4.11. The theoretical line shows $D\lambda/d$ for the given experiment and shows good agreement with the data in Fig. 4.11.

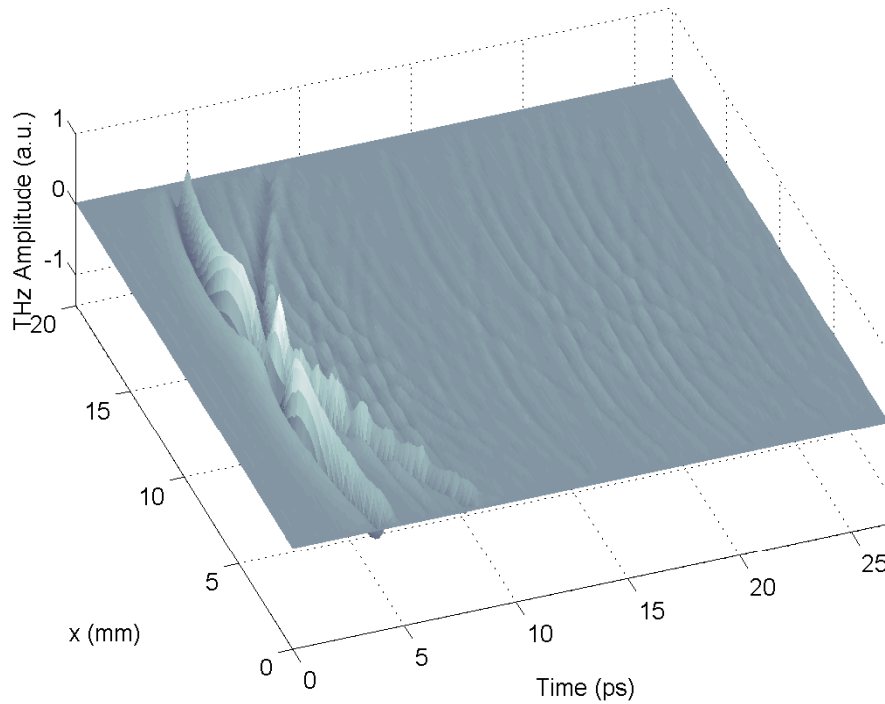


Figure 4.8. THz diffraction pattern caused by Young's double slits. The diffraction pattern measured on the ZnTe sensor is recorded as a function of time. The distribution of the THz intensity as a function of x and time is shown here, where the height is proportional to the relative intensity. The two interfering circular wavefronts are clearly visible. After (Wang et al. 2004).

Reconstructing the Double Slit

The goal of T-ray holography is to reconstruct the spatial aperture of the double slits given the diffraction field measured on the sensor. The method adopted follows that of Ruffin et al. (2001) with two important differences:

1. The reconstruction is performed in the Fourier domain, and
2. Rather than assuming that the distance from the target to the image plane is known *a priori*, an iterative algorithm is developed to estimate this distance.

The first difference is made primarily for computational reasons. Rather than back-propagating the time domain pulses according to the time domain Huygens-Fresnel equation, Eq. (4.7), the frequency domain equivalent for quasi-monochromatic radiation can be used (Sutton 1979, Goodman 1996). The reconstruction formula is

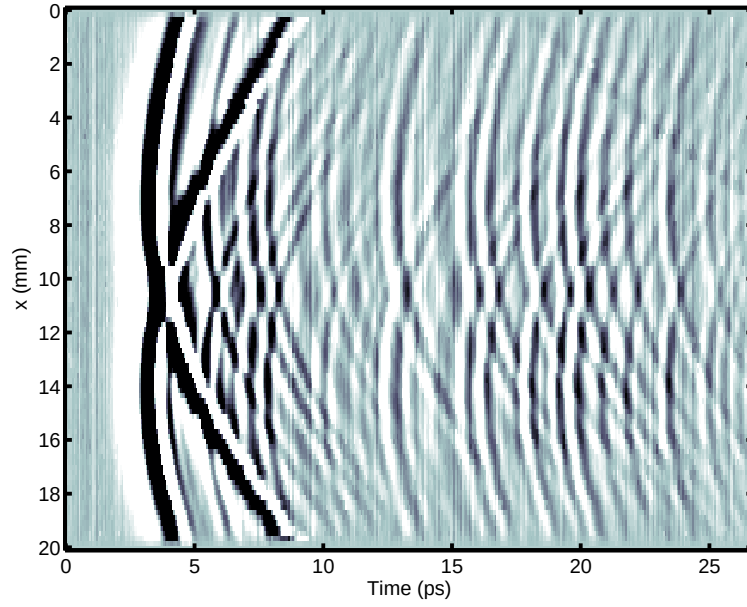


Figure 4.9. Time domain double slit interference pattern. The diffraction pattern is again shown as a function of x and time. In this case a log scale has been used to emphasise the interference pattern after the initial peaks. The interference pattern is complex due to the multiple frequency components present in the THz radiation. After (Wang et al. 2004).

$$U(P_0, \omega) = \frac{1}{i\lambda} \int \int_{M1} U(P_1, \omega) \frac{\exp(-ikr_{01})}{r_{01}} \cos(\hat{n} \cdot r_{01}) ds, \quad (4.10)$$

where λ is the THz wavelength, $M1$ is the measurement plane on the ZnTe sensor surface, P_1 is a point on the measurement plane, P_0 is a point on the reconstructed target plane, r_{01} is the distance between the measurement point on the ZnTe EO sensor and the image point, and $\hat{n}$ is the normal of the measurement plane. Here, $U(P_1, \omega)$ is the Fourier coefficient of the measured THz waveform at frequency $\omega = 2\pi c/\lambda$, and $k = 2\pi/\lambda$ is the propagation number of the radiation.

This equation follows from the Fourier transform of Eq. (4.7) whereby the time delay represented by r_{01}/c becomes a phase shift $\exp(ikr_{01})$. In the frequency domain formulation the backpropagation algorithm simply backpropagates the phase of the Fourier coefficients at each pixel of the sensor according to the distance r_{01} to each position on the target plane and sums them. This is considerably more efficient than translating all the full temporal waveforms.

The reason for this emphasis on computational efficiency is found in the second point noted above. When the separation between the target and sensor planes is known the

4.4 T-ray Holography

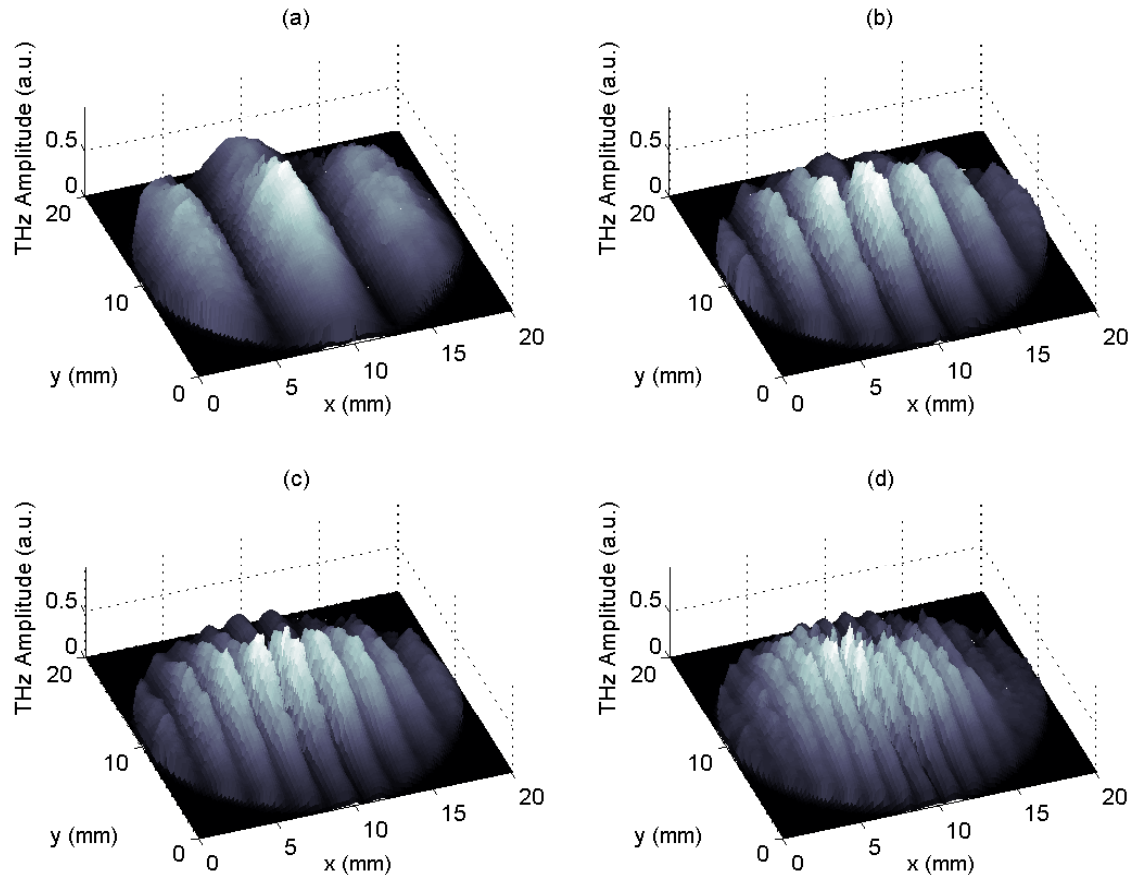


Figure 4.10. Frequency domain double slit interference pattern. The frequency domain diffraction pattern is shown for 4 different frequencies: (a) 0.4 THz, (b) 0.8 THz, (c) 1.2 THz and (d) 1.6 THz. The height of the plots is proportional to the THz intensity. The fringe separation ($D\lambda/d = Dc/fd$) is reduced with increasing frequency.

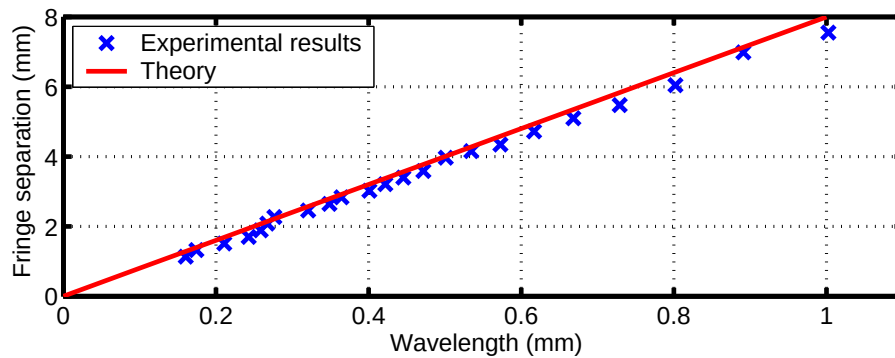


Figure 4.11. Variation of fringe separation with THz wavelength. The fringe separation is measured at each frequency between 150 GHz and 1 THz and is plotted (x). The theoretical line (solid) shows $D\lambda/d$ for the experimental setup. A good agreement with the theory is observed.

backpropagation is a simple linear operation. However, for general inspection operations (in particular for 3D applications, which will be considered shortly) this distance is likely to be unknown and a method was developed to determine this distance independently. This method relies on the fact that the backpropagation operation serves to ‘focus’ the diffracted field back onto the target plane. When the target consists of small apertures in a largely opaque screen this focusing operation will result in maximum intensity at the actual position of the target. Therefore an iterative method was adopted and the backpropagated field is reconstructed at fixed intervals within the practical range. The distance at which the peak radiation intensity is maximised is concluded to be the distance to the target plane. Numerous methods exist to optimise this iterative process however for this concept demonstration a simple step iterative method was adopted.

To demonstrate this method the double slit diffraction data at a frequency of 1 THz was backpropagated according to Eq. (4.10) given a target to sensor distance (D) varying from 42 mm to 54 mm. The peak intensity of the reconstructed field is plotted against distance in Fig. 4.12. The response is well behaved and a quadratic was fitted to the data, yielding good agreement. A significantly faster iterative method can be envisaged where rather than linearly stepping D , a quadratic is fitted to the data at each step and the peak of the fitted quadratic is calculated, and its value used as the next D . This method was implemented and tested. It yielded very fast convergence for the double slit data, however for more general targets it is not guaranteed that the quadratic fit will be accurate.

The reconstructed THz field intensity reached a maximum when D , the distance from the sensor to the target was 47 mm. This is within the measurement error margin of the expected value of 48 mm. Once D was known the reconstructed slit profile could be determined and this is shown in Figs. 4.13 and 4.14. Figure 4.13 shows the reconstructed 1D cross-section of the THz intensity at the slits. The slit separation is 7 mm and the width of the slits (at half the maximum amplitude) are 1.2 mm and 1 mm respectively. This reconstruction shows good agreement with the expected geometry shown in Fig. 4.7. The 2D reconstruction was also performed and is shown in Fig. 4.14. The reconstructed field tapers off towards the edges of the reconstructed region due to the limited angular aperture. This effect is clearly seen at the top and bottom of the reconstructed slits.

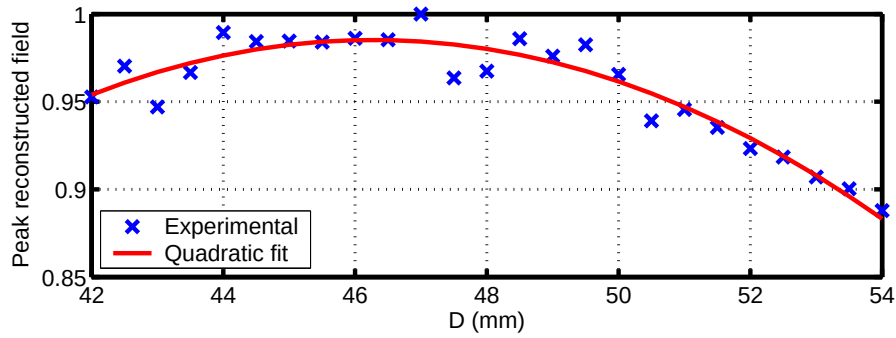


Figure 4.12. Variation of peak intensity with target to sensor distance. Backpropagation of the Fresnel diffraction equation was used to reconstruct the spatial aperture pattern of the double slits. The distance from the slits to the sensor (D) was assumed to be an unknown and the reconstruction was performed iteratively for D ranging between 42 mm and 54 mm with a step size of 0.5 mm. The peak intensity of the reconstructed field is plotted against distance ($\times$). The intensity reaches a maximum at the actual D . A quadratic was fitted to the data (solid line) and shows good agreement with the results.

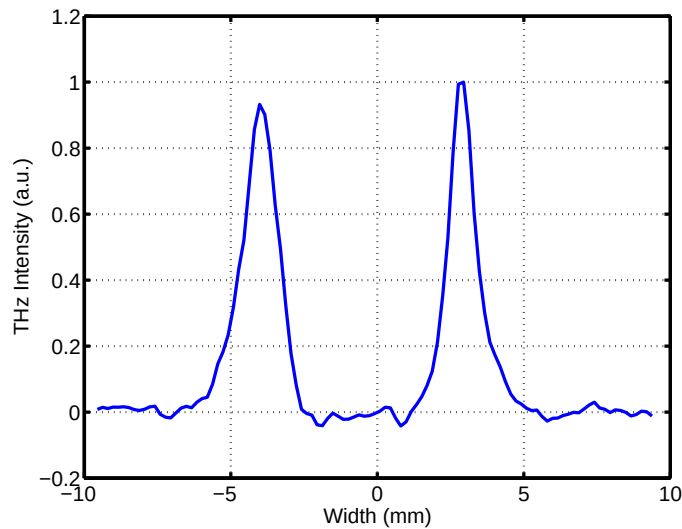


Figure 4.13. Double slit profile reconstructed using Fresnel backpropagation. The diffraction data at a frequency of 1 THz was backpropagated according to Eq. (4.10) using $D = 47$ mm as estimated using the iterative method described in the text. The data was averaged in the y dimension to allow the horizontal cross-section to be reconstructed with high SNR. The reconstructed slits have a slit width of 1.2 mm and 1 mm and a separation of 7 mm in close agreement with the expected results (1 mm, 1 mm and 6 mm respectively).

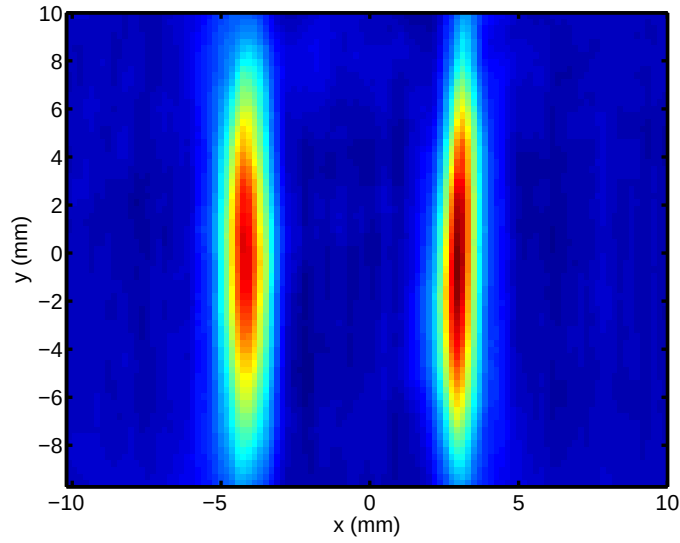


Figure 4.14. 2D double slit image reconstructed using Fresnel backpropagation. The diffraction data at a frequency of 1 THz was backpropagated according to Eq. (4.10) using $D = 47$ mm as estimated using the iterative method described in the text. A 2D reconstruction was performed and the slits are clearly visible. The intensity of the reconstruction falls at the top and bottom of the reconstructed image as a result of the limited extent of the sensor crystal.

The technique of 2D T-ray holography is significant for a number of reasons. Firstly the measurement method is several orders of magnitude faster than previous backpropagation techniques, which makes real-time operation and real-world imaging applications plausible. Secondly, it reveals the fact that targets can be accurately reconstructed despite the fact that the diffracted radiation is only acquired over a very limited angular aperture. Finally this method forms the basis for a novel 3D holography method considered in the next section.

4.4.3 3D T-ray Holography

To investigate the extension of this holography system to 3D imaging a simple target consisting of point scatterers was considered. The hardware schematic is illustrated in Fig. 4.15. A plane Gaussian THz beam propagates through samples S_1 and S_2 and is reflected towards the ZnTe electro-optic (EO) sensor by an ITO THz mirror. The optical probe beam is transmitted through the ITO glass and propagates collinearly with the THz beam. The probe beam is modulated by the THz diffraction pattern at the ZnTe EO sensor through the EO effect (Wu et al. 1996), thereby transferring the THz wave

4.4 T-ray Holography

diffraction pattern onto the probe beam. By changing the time delay between probe and THz beams, the temporal THz diffraction pattern carried by the probe beam at each time delay is recorded using a lens and a CCD.

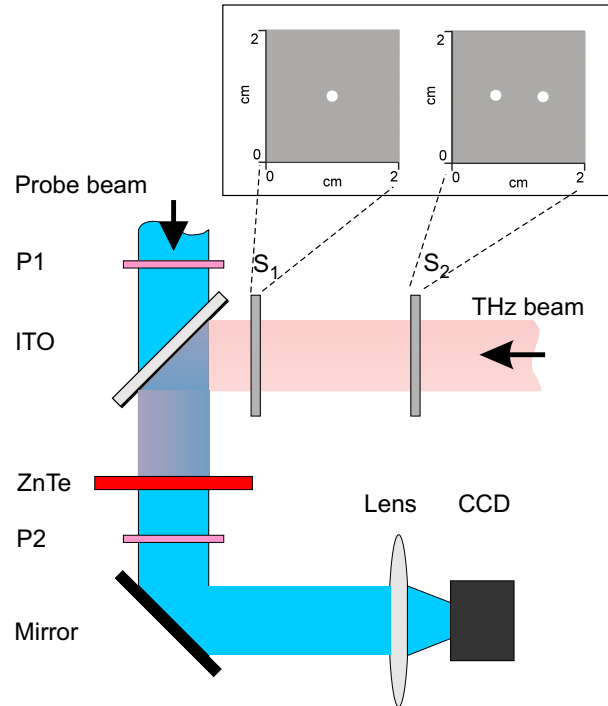


Figure 4.15. Experimental setup for three-dimensional terahertz digital holography. A planar Gaussian THz beam with a diameter of 2.5 cm ($1/e$) propagates through samples S_2 and S_1 and is reflected by an ITO THz mirror. An optical probe beam with the same diameter propagates collinearly with the THz beam towards a ZnTe EO sensor. After the propagating through the ZnTe and analyser P2, the probe beam is focused onto CCD. The polarisation direction of the polariser P1 and that of the analyser P2 are perpendicular to each other. The top inset shows the front view of S_1 and S_2 . After (Wang et al. 2004).

The target consisted of two 3.5 mm thick polyethylene plastic sheets, samples S_1 and S_2 . Small holes were drilled into each sheet such that the holes acted as point scatterers. The optical distances from S_1 and S_2 to the ZnTe sensor were 4.5 cm and 9 cm respectively. The separation between the holes on each sample (6 mm) was much larger than the peak wavelength of the THz beam (0.3 mm), and the hole diameters were 1.8 mm. There are multiple scattering paths through the target. When the THz wave propagates through a hole, it arrives at an earlier time delay compared with the wave propagating through the plastic sheets. For ease of reference the wave propagating through the holes will be referred to as the scattered THz wave.

At each pixel of the CCD the THz temporal waveform was recorded. The response at the centre pixel is shown in Fig. 4.16. The waveform at every pixel displays three distinct pulses, w_1 , w_2 and w_3 , which start at around 3.4 ps, 9.2 ps and 15 ps, respectively. Additional information may be inferred by considering the timing of these pulses as a function of sensor position. Figure 4.17 shows the measured THz wave front along three lines labeled A, B and C on the ZnTe crystal respectively. Pulse w_3 arrives at the longest delay and its timing is largely invariant of the sensor position. It corresponds to the non-scattered THz plane wave transmitted through both plastic sheets S_1 and S_2 . Pulse w_1 arrives at the earliest time delay and results from the waves that are multiply scattered by the holes of both S_1 and S_2 samples. Pulse w_2 is a superposition of the waves that are scattered once by the holes of either S_1 or S_2 . As seen in Fig. 4.16 the scattered waves w_1 and w_2 are weak compared to the non-scattered wave. By windowing the THz waveform it is possible to obtain the 'localised pulse' that contains the 'local hologram', which results from the scattered waves caused by a single plane of the target. For example, the window shown in Fig. 4.16 can be used to isolate the 'localised pulse' w_2 . The windowed Fourier transform of this 'localised pulse' provides amplitude and phase information as a function of frequency that may be used to reconstruct the target.

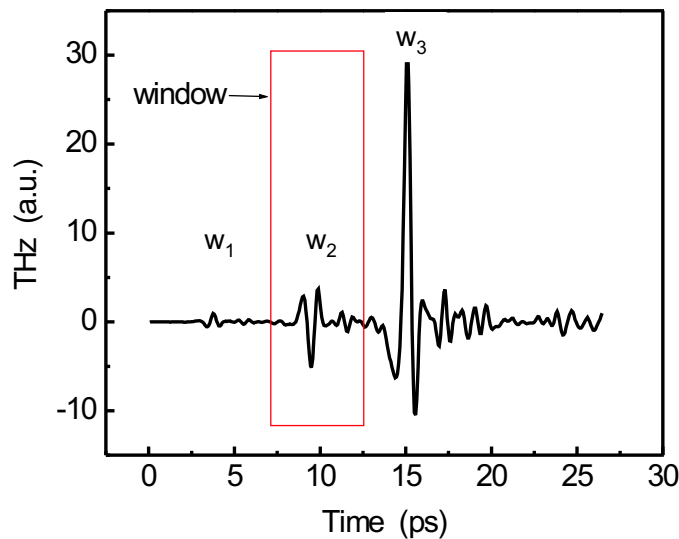


Figure 4.16. The THz waveform measured at the centre of the ZnTe sensor. The waveform shows three distinct pulses, termed w_1 , w_2 and w_3 . If we apply a window to the waveform, it is possible to separate the waves that experienced different scattering paths.

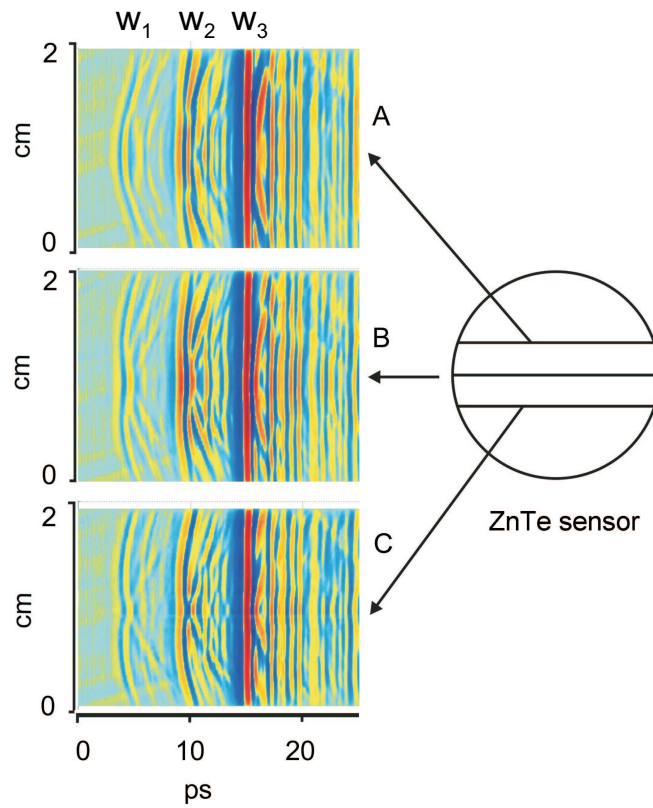


Figure 4.17. Wave front images of the diffracted THz wave along three horizontal lines across the ZnTe EO sensor. Line B is a diameter, lines A and C are chords parallel to B, 3 mm above and below the centre line B. All the wave fronts show three distinct parts, w_1 , w_2 and w_3 , which start at approximately 3.4 ps, 9.2 ps and 15 ps respectively, their separations in time correspond to the thickness of the polyethylene sheets. After (Wang et al. 2004).

4.4.4 Windowed Fourier Transform

Fourier analysis is ideal for analysing stationary periodic signals. However, it is of limited use when processing non-stationary signals because the frequency information is extracted for the complete duration of the measured signal, while the event of interest may occur within a short, specific duration. A solution for studying such local spectra is to truncate the wave in the specific region and perform the discrete Fourier transformation (DFT), this is referred to as the windowed Fourier transformation (WFT) (Kaiser 1994, Carin et al. 1997).

The Fourier transform $F(\omega)$ of a continuous function $f(t)$ is defined as

$$F(\omega) = \int_{-\infty}^{+\infty} f(t)e^{-i\omega t} dt. \quad (4.11)$$

The windowed Fourier transformation is given by

$$F(\omega) = \int_{-\infty}^{+\infty} g(t)f(t)e^{-i\omega t}dt. \quad (4.12)$$

where $g(t)$ is the window function. A number of windows are available. The simplest is the rect function, with a width τ and centred at time t_1 ,

$$g(t) = \text{rect}\left[\frac{(t - t_1)}{\tau}\right] = \begin{cases} 1 & \text{if } |t - t_1| < \tau/2 \\ 0 & \text{if } |t - t_1| \geq \tau/2. \end{cases} \quad (4.13)$$

The discrete analog of the WFT was applied to the ‘localised pulses’ to calculate the frequency-domain diffraction pattern generated by each pulse. Given the measured diffraction pattern, a 2D reconstruction of the spatial scattering centre distribution can be performed using the backpropagation method discussed in Sec. 4.4.2.

4.4.5 Reconstruction Algorithm

A 3D reconstruction algorithm can be devised by iteratively considering each of the localised pulses w_1 , w_2 and w_3 . It commences by analysing the hologram formed by pulse w_1 . A window is set to capture w_1 and the WFT is performed. Using the field components at a frequency of 1 THz the field distribution at sample S_1 is reconstructed using Eq. (4.10). By analysing the timing of the pulses, it can be shown that w_1 consists of the doubly scattered wave that passed through the holes in S_1 and S_2 . Provided the planes are well separated the diffracted field w_1 will only include information on the latest scattering plane S_1 . Therefore backpropagating this field yields the location of the scattering centres in S_1 , the reconstructed estimate of the spatial distribution of S_1 is denoted $\hat{S}_1$. To implement Eq. (4.10) requires knowledge of the distance (along the beam propagation direction) between the sensor and the target plane. In many holographic applications this distance is known *a priori*, however in general inspection applications it is unknown. This problem is overcome by performing the reconstruction at multiple distances and choosing the distance at which the reconstructed field is maximised as discussed in Sec. 4.4.2. This method is successful for this target as the backpropagation algorithm serves to ‘focus’ the diffracted radiation back on the target plane, and for a series of point scatterers the field is maximised when the scatterers are in focus. An alternative method is to use the curvature of the spherical waves seen in Fig. 4.17 since the radius of curvature of the spherical waves is equal to the distance to

the target plane. Methods of extending these techniques to more general targets are an important future research focus.

Once $\hat{S}_1$ is determined, the second pulse w_2 and its corresponding backpropagated hologram are considered. The procedure is similar to the reconstruction procedure for w_1 , a window is calculated to capture the pulse w_2 and the Windowed Fourier Transformation is performed. An additional processing stage is required because w_2 contains two contributions, one from S_1 and another from S_2 . The simple backpropagated hologram would therefore be a superposition of two diffraction patterns resulting from S_1 and S_2 respectively. Since the reconstruction $\hat{S}_1$ is already known, the THz plane wave w_3 (assumed to be the incident field) may be forward propagated (using the Fresnel-Kirchhoff formula) through the reconstructed $\hat{S}_1$ to estimate the contribution of S_1 to w_2 . This is then subtracted from w_2 and the remainder may be backpropagated to determine $\hat{S}_2$. This procedure is elucidated more clearly mathematically. To do so we define two complementary operators, the backpropagation operator G^{BP} , which implements Eq. (4.10) such that $U(P_0) = G_r^{BP}U(P_1)$, and its inverse: a forward propagation operator $G^{FP} : U(P_1) = G_r^{FP}U(P_0)$, where r is the perpendicular distance between the sensor and target planes. We assume that w_3 is approximately equal to the input wave w_0 , and denote the complex THz field amplitudes at the detector plane arising from w_1 , w_2 and w_3 as U_{w_1} , U_{w_2} and U_{w_3} respectively. It follows that:

$$U_{w_1} = G_{d_1}^{FP} \left[S_1 \cdot G_{d_2}^{FP} (S_2 \cdot U_{w_0}) \right], \quad (4.14)$$

$$U_{w_2} = G_{d_1+d_2}^{FP} (S_2 \cdot U_{w_0}) + G_{d_1}^{FP} (S_1 \cdot U_{w_0}), \quad (4.15)$$

$$\hat{S}_1 = G_{d_1}^{BP} U_{w_1}, \quad (4.16)$$

$$\hat{S}_2 = G_{d_1+d_2}^{BP} \left[U_{w_2} - G_{d_1}^{FP} (\hat{S}_1 \cdot U_{w_3}) \right], \quad (4.17)$$

where S_1 and S_2 are binary spatial masks matching the geometry of the targets, d_2 is the perpendicular distance between S_1 and S_2 , d_1 is the perpendicular distance between S_1 and the sensor, and $\hat{x}$ indicates the estimated value of x . If there are point scatterers on more than two target planes additional pulses will be observed in the THz response and this reconstruction algorithm may be extended by applying additional steps for each target plane.

4.4.6 Experimental Results

The reconstructed images of $\hat{S}_1$ and $\hat{S}_2$ are shown in Fig. 4.18 (c) and (d). The reconstructed distances from S_1 and S_2 to ZnTe sensor were found to be 4.6 cm and 9.3 cm respectively, in good agreement with the actual separations of 4.5 cm and 9 cm. The reconstructed images show excellent correspondence with the target geometry, as shown in Fig. 4.18 (a) and (b), although the holes in the far plane S_2 are slightly blurred. Figure 4.19 shows an additional reconstruction of two slightly more complex samples using the same procedure. Again a good agreement with the expected result was observed.

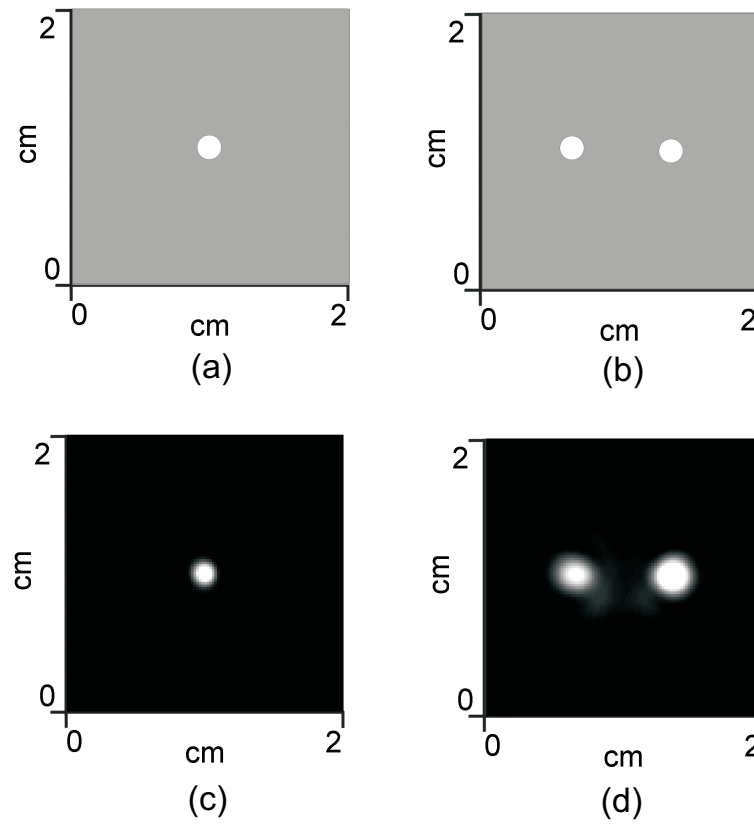


Figure 4.18. Schematic of simple holography target samples and their reconstructed holograms. (a) Schematic of sample S_1 , (b) Schematic of sample S_2 , (c) Reconstructed hologram of S_1 , (d) Reconstructed hologram of S_2 . The reconstructed image distances from the ZnTe sensor were 4.4 cm and 9.2 cm respectively. After (Wang et al. 2004).

Resolution

It is worth considering the resolution of this holography method. Since the backpropagation method serves to effectively ‘focus’ the diffracted field back to the target we may expect that the resolution would be diffraction limited according to the commonly used

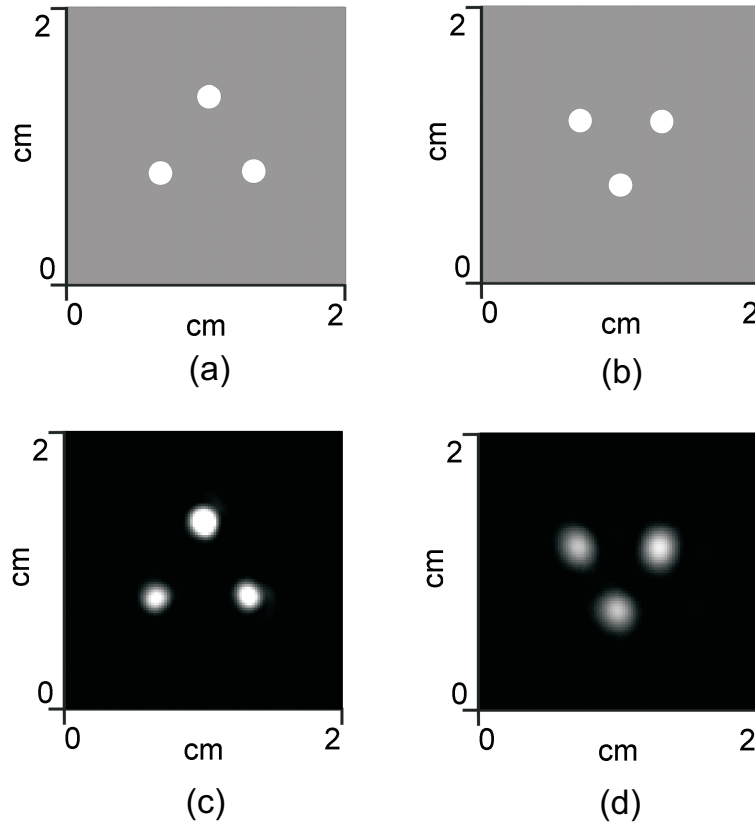


Figure 4.19. Schematic of holography target samples and their reconstructed holograms. (a) Schematic of sample S_1 , (b) Schematic of sample S_2 , (c) Reconstructed hologram of S_1 , (d) Reconstructed hologram of S_2 . The reconstructed image distances from the ZnTe sensor were 4.6 cm and 9.3 cm respectively. After (Wang et al. 2004).

Rayleigh criterion. By considering the backpropagation operation to be comparable to a simple lens focusing the radiation the resolution can be expressed by

$$\delta x = \frac{1.22\lambda f}{D}, \quad (4.18)$$

where δx is the resolution, λ is the wavelength at which the reconstruction is performed, f is the focal length corresponding to the distance between the sensor and target planes and D is the ‘aperture’ of the ‘lens’ that corresponds to the diameter of the detector crystal. For the Young’s double slit experiment from Sec. 4.4.2, where $\lambda = 0.3$ mm, $f = 47$ mm and $D = 20$ mm, the expected resolution is 0.86 mm. The 10-90% rise time for the reconstructed double slit is 0.9 mm, indicating that Eq. (4.18) is a reasonable approximation. The resolution is degraded as the target is moved further away. This is observed clearly in Fig. 4.19 where the holes in the more distant plane S_2 are blurred. The resolution can be improved by increasing the size of the sensor or performing the reconstruction at a higher frequency.

4.4.7 Summary

T-ray holography provides high fidelity images for targets consisting of point scatterers located on well-separated planes. However it has a number of pertinent deficiencies. Its extension to more complex targets is far from trivial, and in any case it does not provide accurate refractive index data on the reconstructed target and is therefore of little use for material identification. A goal of this Thesis is the development of methods providing the capability for spectroscopic identification of different materials. The next section considers the first of such methods.

4.5 T-ray Diffraction Tomography

In the previous section, T-ray holography was explored whereby the Fresnel diffraction equation was adopted as the model for THz-wave propagation. This equation is derived under an assumption of homogenous free space wave propagation, which gives rise to the restriction to point scatterer-based targets. In contrast, T-ray diffraction tomography (Devaney 1982, Mueller et al. 1980, Pan and Kak 1983, Testorf and Fiddy 1999, Mast et al. 1999, Carney et al. 1999) adopts the Helmholtz equation, which describes electromagnetic wave propagation in more general media. T-ray diffraction tomography is based on linearised inverse scattering techniques borrowed from RF and ultrasound tomography systems.

4.5.1 Wave Propagation Theory

The goal of T-ray diffraction tomography is to determine the spatial distribution of a target's refractive index using measurement of the diffracted THz field. The relationship between the THz wave distribution and the target's refractive index as a function of position, $\mathbf{r}$ can be described by Maxwell's equations (Born and Wolf 1999),

$$\nabla^2 \mathbf{E} + \frac{\mu(\mathbf{r})\epsilon(\mathbf{r})}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} + [\nabla \ln \mu(\mathbf{r})] \times (\nabla \times \mathbf{E}) + \nabla[\mathbf{E} \cdot \nabla \ln \epsilon(\mathbf{r})] = 0, \quad (4.19)$$

where c is the speed of light in a vacuum, $\mathbf{E}$ is the vector electric field and $\epsilon(\mathbf{r})$ and $\mu(\mathbf{r})$ are the complex dielectric constant function and magnetic permeability, respectively. If ϵ and μ vary slowly over a wavelength of the input electromagnetic wave, $\nabla \ln \epsilon(\mathbf{r}) = \nabla \ln \mu(\mathbf{r}) \approx 0$, and Eq. (4.19) can be reduced to

$$\nabla^2 \mathbf{E} + \frac{\tilde{n}(\omega, \mathbf{r})^2}{c^2} \frac{\partial^2}{\partial t^2} \mathbf{E} = 0, \quad (4.20)$$

4.5 T-ray Diffraction Tomography

where $\tilde{n}(\mathbf{r}) = \sqrt{\epsilon(\mathbf{r})\mu(\mathbf{r})}$ is the refractive index of the medium. Neglecting polarisation effects, and transforming to the frequency, ω , domain, Eq. (4.20) can be written as the scalar Helmholtz equation

$$\nabla^2 u(\mathbf{r}) + k_0^2 \tilde{n}(\omega, \mathbf{r})^2 u(\mathbf{r}) = 0, \quad (4.21)$$

where $u(\mathbf{r})$ is the electromagnetic field complex amplitude function, and $k_0 = 2\pi/\lambda$ is the propagation number of the electromagnetic wave in a vacuum. The Helmholtz equation is valid in a wide range of applications (Ishimaru 1978), and it forms the basis of the following 3D imaging techniques. Our goal is to determine a target's refractive index function $\tilde{n}(\mathbf{r})$, given the measured THz wave amplitude and phase distribution $u(\mathbf{r})$, this problem is referred to as the Inverse Scattering Problem (ISP) (Baltes 1978). Equation (4.21) may be written as

$$(\nabla^2 + k_0^2)u(\mathbf{r}) = -o(\mathbf{r})u(\mathbf{r}), \quad (4.22)$$

where $o(\mathbf{r})$ is the target's object function, given by

$$o(\mathbf{r}) = -k_0^2[\tilde{n}(\omega, \mathbf{r})^2 - 1]. \quad (4.23)$$

The solution of Eq. (4.23), $u(\mathbf{r})$, can be considered to be the sum of two components,

$$u(\mathbf{r}) = u_0(\mathbf{r}) + u_s(\mathbf{r}), \quad (4.24)$$

where, $u_s(\mathbf{r})$ is the scattered field caused by the target and $u_0(\mathbf{r})$ is the incident field, the field that would be present without a target, or, equivalently, a solution to the homogenous Helmholtz equation,

$$(\nabla^2 + k_0^2)u_0(\mathbf{r}) = 0. \quad (4.25)$$

Combining Eq. (4.25), Eq. (4.24) and Eq. (4.22) yields a wave equation for the scattered component

$$(\nabla^2 + k_0^2)u_s(\mathbf{r}) = -o(\mathbf{r})u(\mathbf{r}). \quad (4.26)$$

The solution to Eq. (4.26) can be written in terms of the Green's function (Morse and Feshbach 1953)

$$u_s(\mathbf{r}) = u_0(\mathbf{r}) + \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u(\mathbf{r}')d\mathbf{r}', \quad (4.27)$$

where the Green's function is the solution of the differential equation,

$$(\nabla^2 + k_0^2)G(\mathbf{r} - \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'), \quad (4.28)$$

where $\delta(\mathbf{r} - \mathbf{r}')$ is the Dirac delta function. In three dimensions the Green's function is given by

$$G(\mathbf{r} - \mathbf{r}') = \frac{\exp(ik_0|\mathbf{r} - \mathbf{r}'|)}{4\pi|\mathbf{r} - \mathbf{r}'|}, \quad (4.29)$$

while in two dimensions it is expressed in terms of the zero-order Hankel function of the 1st kind, $H_0^{(1)}$,

$$G(\mathbf{r} - \mathbf{r}') = \frac{i}{4}H_0^{(1)}(k_0|\mathbf{r} - \mathbf{r}'|). \quad (4.30)$$

Equation (4.27) provides a solution for $u_s(\mathbf{r})$, in the terms of total field, which in turn depends on the scattered field, $u(\mathbf{r}) = u_0(\mathbf{r}) + u_s(\mathbf{r})$. This equation must still be solved for the scattered field, for this problem we turn to the Born and Rytov approximations (Kak and Slaney 2001).

The First Born Approximation

The Born approximation was introduced by Max Born in 1925 as a technique for solving the Schrödinger equation in the field of atomic physics (Born and Jordan 1925). Equation (4.27) can be expanded as a Born series

$$u(\mathbf{r}) = u_0(\mathbf{r}) + \sum_{j=1}^i u_j(\mathbf{r}), \quad (4.31)$$

where the sum is referred to as the i th order Born approximation, and $u_j(\mathbf{r})$ is the j th-order scattered field,

$$u_j(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_{j-1}(\mathbf{r}')d\mathbf{r}'. \quad (4.32)$$

If the scattered field $|u_s(\mathbf{r})|$ is much smaller than the incident field $|u_0(\mathbf{r})|$, the scattered field can be approximated by the first-order scattered field ($i = 1$), this is referred to as the first Born approximation,

$$u_s(\mathbf{r}) = u_1(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_0(\mathbf{r}')d\mathbf{r}'. \quad (4.33)$$

In deriving the first Born approximation it is assumed that the scattered field is much smaller than the incident field. For certain targets it is possible to translate this condition into a derivation of the target properties required for the Born approximation to be valid. For plane wave illumination of a cylinder with refractive index n and radius a , Kak and Slaney (2001) showed that this condition implies that

$$a(\tilde{n} - 1) < \frac{\lambda}{4}. \quad (4.34)$$

The First Rytov Approximation

The Rytov approximation (Rytov 1938) offers an alternative linearisation of the wave equation. It assumes that the incident wave perturbation caused by the target can be described by a change of phase in the reference wave. It is derived by considering the total field to be represented as complex phase (Ishimaru 1978)

$$u(\mathbf{r}) = e^{\phi(\mathbf{r})} = e^{\phi_0(\mathbf{r}) + \phi_s(\mathbf{r})}. \quad (4.35)$$

Combining Eq. (4.26), Eq. (4.25) and Eq. (4.35) and reducing the resultant expressions (Kak and Slaney 2001) yields

$$(\nabla^2 + k_0^2)u_0(\mathbf{r})\phi_s(\mathbf{r}) = -u_0(\mathbf{r})[(\nabla\phi_s(\mathbf{r}))^2 + o(\mathbf{r})]. \quad (4.36)$$

The first Rytov approximation assumes that the gradient of the scattered complex phase $\phi_s(\mathbf{r})$ is small, therefore

$$(\nabla\phi_s(\mathbf{r}))^2 + o(\mathbf{r}) \approx o(\mathbf{r}). \quad (4.37)$$

The solution for the scattered phase $\phi_s(\mathbf{r})$ is then

$$u_0(\mathbf{r})\phi_s(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_0(\mathbf{r}')d\mathbf{r}'. \quad (4.38)$$

The complex phase of the scattered field is therefore given by

$$\phi_s(\mathbf{r}) = \frac{1}{u_0(\mathbf{r})} \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_0(\mathbf{r}')d\mathbf{r}'. \quad (4.39)$$

The Born and Rytov approximations both result in solutions to Eq. (4.21) that have the same form, the solution is proportional to a convolution of the Green's function with the product of the object function and the incident wave.

The Rytov approximation is more accurate than the Born approximation, especially at higher frequencies (Devaney 1983). However, for small, low contrast targets the two approximations are equivalent. If $\phi_s(\mathbf{r}) \ll 1$, then $e^{\phi_s(\mathbf{r})} \approx 1 + \phi_s(\mathbf{r})$ and we observe that

$$\begin{aligned} u(\mathbf{r}) &= e^{\phi_0(\mathbf{r}) + \phi_s(\mathbf{r})}, \\ &= u_0(\mathbf{r})e^{\phi_s(\mathbf{r})}, \\ &\approx u_0(\mathbf{r})[1 + \phi_s(\mathbf{r})], \\ &= u_0(\mathbf{r}) + \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_0(\mathbf{r}')d\mathbf{r}', \end{aligned} \quad (4.40)$$

which yields the first Born approximation.

The condition for the applicability of the Rytov approximation is less restrictive than the Born approximation. It assumes that $o(\mathbf{r}) \gg (\nabla\phi_s)^2$ as shown in Eq. (4.37). To a first approximation $o(\mathbf{r})$ is proportional to n_δ , where n_δ is defined as $n_\delta = \tilde{n} - 1$, in fact $o(\mathbf{r}) \approx 2k_0^2 n_\delta(\mathbf{r})$. This implies that

$$n_\delta \gg \frac{[\nabla\phi_s(\mathbf{r})]^2}{k_0^2}, \quad (4.41)$$

$$\gg \frac{[\nabla\phi_s(\mathbf{r})\lambda]^2}{(2\pi)^2}. \quad (4.42)$$

In other words, the Rytov approximation requires that the phase of the scattered field varies slowly relative to one wavelength. The size of the target is therefore less critical under the Rytov approximation.

These approximations to the Helmholtz equation allow linear reconstruction algorithms to be developed to reconstruct the target's object function, $o(\mathbf{r})$, based on measurements of the diffracted radiation from multiple projections.

4.5.2 T-ray Diffraction Tomography System

To acquire the required diffraction data a T-ray diffraction tomography system was developed (Ferguson et al. 2002c). The T-ray DT system is based on the 2D electro-optic sampling imaging system and utilises synchronised dynamic subtraction and sensor calibration to provide a sufficient SNR. The imaging system is described in detail in Sec. 3.3.2. The sample is mounted on a computer controlled rotation stage and positioned 50 mm from the ZnTe detector. The T-ray DT schematic is shown in Fig. 4.20. A PCA THz emitter was used to maximise the THz power and SNR. The Born and Rytov approximations restrict the targets that may be considered to those with a relatively small refractive index. This implies that the scattered field has relatively small amplitude and necessitates a system with high SNR. The PCA used had an electrode spacing of 16 mm and a bias voltage of 2 kV was applied.

A single motion stage is required to scan the THz temporal profile and the target is rotated to obtain an image at multiple projection angles. The minimum data acquisition period for a CCD exposure time of 15 ms per frame and a projection step size of 10° is approximately 8 minutes. However, in practice, multiple CCD frames are averaged to improve the SNR.

4.5 T-ray Diffraction Tomography

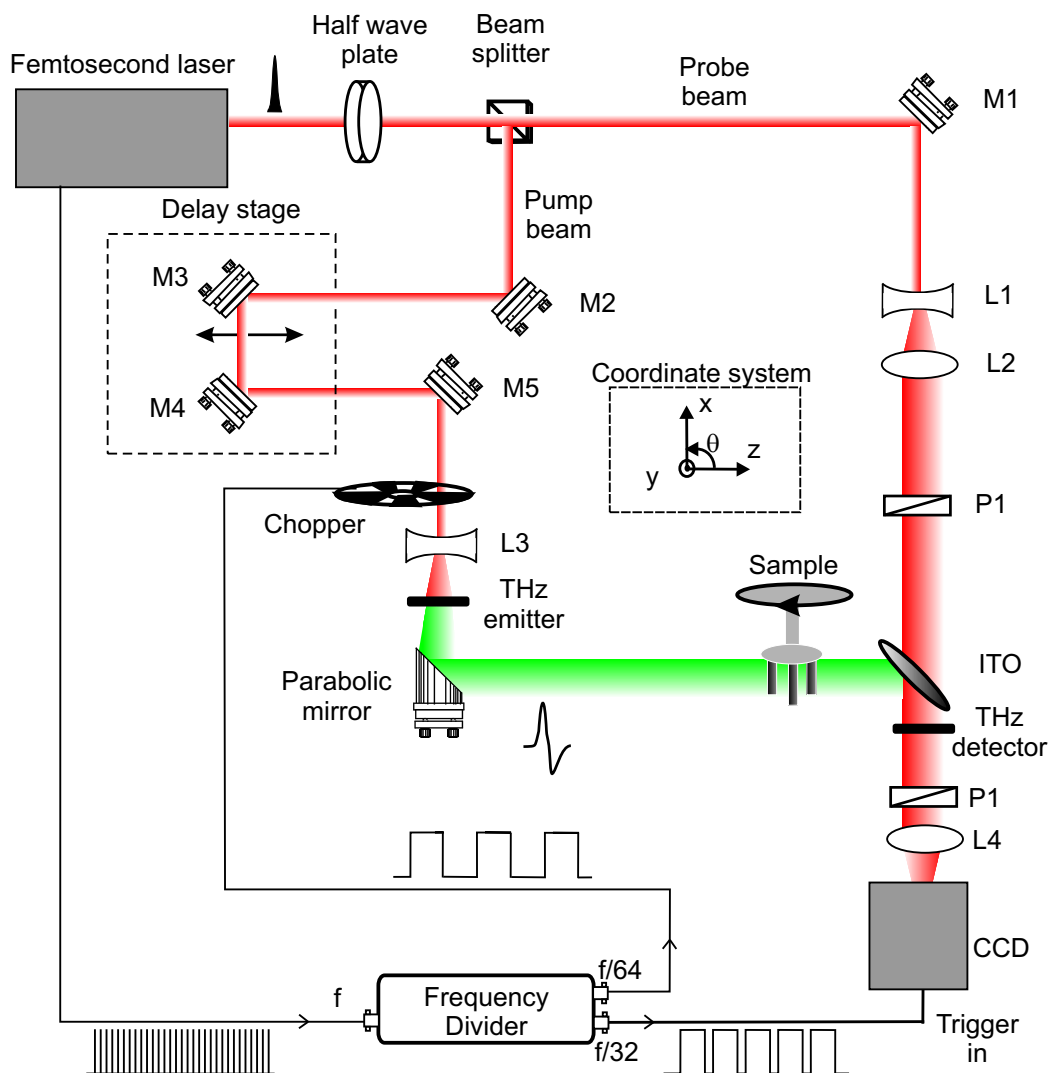


Figure 4.20. Hardware schematic for T-ray diffraction tomography. The system is based on the 2D FSEOS system described in Sec. 3.3.2. Synchronised dynamic subtraction is used to improve the SNR. The THz wave is diffracted as it interacts with the sample and the diffraction pattern is measured on the CCD. The sample is mounted on a rotation stage allowing it to be rotated in the $x - z$ plane and the diffraction field measured for multiple projection angles θ .

4.5.3 Reconstruction Algorithm

The scattered THz field caused by the target was measured and an algorithm was sought to allow the target's structural information to be recovered. Neglecting polarisation, the THz electric field satisfies the wave equation of Eq. (4.26). The reconstruction is performed in the frequency domain, by Fourier transforming the measured THz time domain pulses and using the Fourier coefficients at a single frequency. Given the first order approximations described in Sec. 4.5.1 the scattered field distribution is

$$\phi_s(\mathbf{r})u_0(\mathbf{r}) = u_s(\mathbf{r}) = \int G(\mathbf{r} - \mathbf{r}')o(\mathbf{r}')u_0(\mathbf{r}')d\mathbf{r}'. \quad (4.43)$$

The goal of diffraction tomography is to invert this equation to calculate the object function, $o(\mathbf{r})$. The solution to this problem is found in the Fourier Diffraction Theorem, which states that:

When an object, $o(x, z)$, is illuminated with a plane wave as shown in Fig. 4.21, the Fourier transform of the forward scattered field measured on the line TT' gives the values of the 2-D transform, $O(u, v)$, of the object along a semicircular arc in the frequency domain, as shown in the right half of the figure.

- (Kak and Slaney 2001)

The Fourier Diffraction Theorem may be derived by considering the experimental configuration shown in Fig. 4.22. An object $o(\mathbf{r})$ is illuminated with a single plane wave represented by

$$u_0(\mathbf{r}) = \exp(ik \cdot \mathbf{r}) \quad (4.44)$$

where $\mathbf{k}$ is the wave vector composed of the wave vector coefficients $\hat{\alpha}$ and $\hat{\gamma}$ in the directions (x, z) , and $k_0^2 = \hat{\alpha}^2 + \hat{\gamma}^2$.

The forward scattered field is measured on a line perpendicular to the direction of incidence at $z = d$.

The Green's function in Eq. (4.43) is given by Eq. (4.30). The plane wave decomposition of this function is given by (Kak and Slaney 2001)

$$G(\mathbf{r} - \mathbf{r}') = \frac{i}{4\pi} \int \int \frac{1}{\hat{\gamma}} \exp[i\hat{\alpha}(x - x') + i\hat{\gamma}(z - z')]d\hat{\alpha}, \quad (4.45)$$

Inserting Eq. (4.45) into Eq. (4.43) yields

$$u_s(\mathbf{r}) = \frac{i}{4\pi} \int o(\mathbf{r}')u_0(\mathbf{r}') \int \frac{1}{\hat{\gamma}} \exp \{i [\hat{\alpha}(x - x') + \hat{\gamma}|z - z'|]\} d\hat{\alpha}d\mathbf{r}'. \quad (4.46)$$

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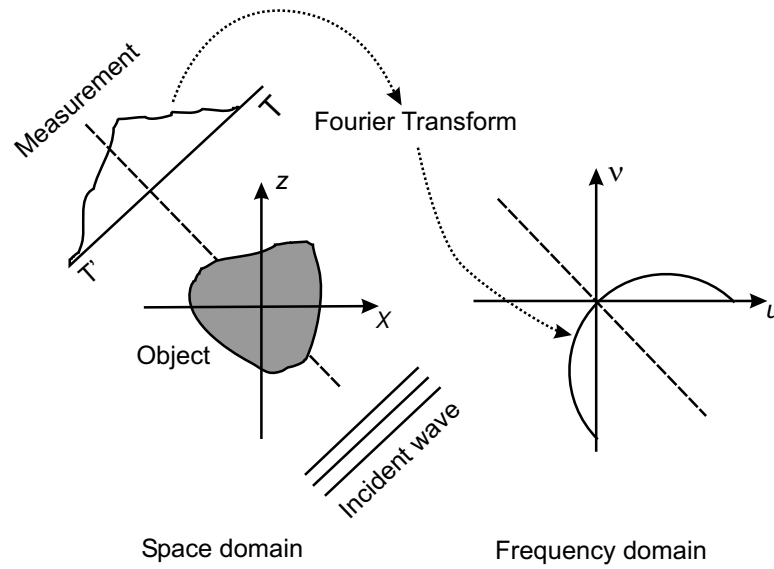


Figure 4.21. The Fourier Diffraction Theorem in two dimensions. The Fourier Diffraction Theorem relates the Fourier transform of a diffracted projection to the Fourier transform of the object along a semicircular arc. After (Kak and Slaney 2001).

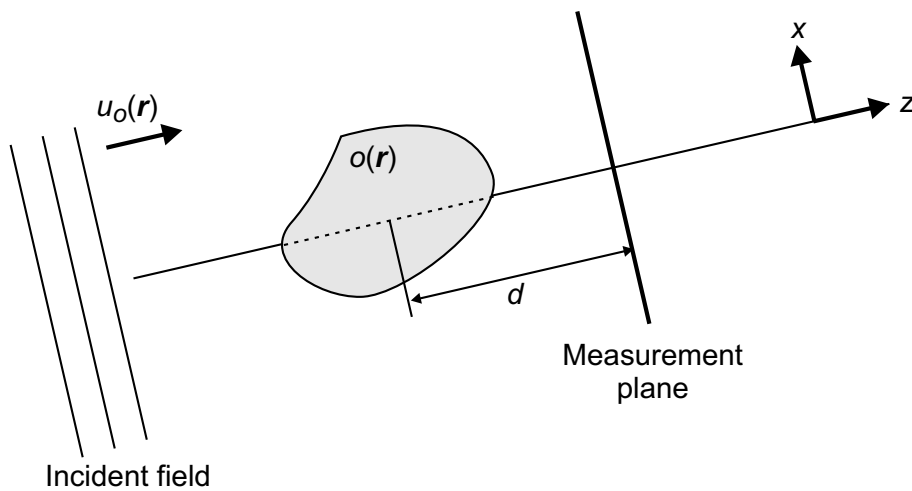


Figure 4.22. The classical diffraction tomography measurement configuration. A plane wave is scattered by the object $o(r)$; the scattered wave is measured on a plane perpendicular to the incident wave vector, located a distance d from the target. The co-ordinate system is chosen with z along the axis of the incident wave vector.

Considering the geometry described in Fig. 4.22, Eq. (4.46) becomes

$$u_s(x, z = d) = \frac{i}{4\pi} \int d\hat{\alpha} \int \frac{o(\mathbf{r}')}{\hat{\gamma}} \exp \{i [\hat{\alpha}(x - x') + \hat{\gamma}(d - z')]\} \exp \{ik_0 z'\} d\mathbf{r}'. \quad (4.47)$$

The inner integral of Eq. (4.47) may be recognised as the two-dimensional Fourier transform of the object function evaluated at a frequency of $(\hat{\alpha}, k_0 - \hat{\gamma})$. Thereby

$$u_s(x, z = d) = \frac{i}{4\pi} \int \frac{1}{\hat{\gamma}} \exp \{i [\hat{\alpha}x + \hat{\gamma}d]\} O(\hat{\alpha}, \hat{\gamma} - k_0) d\hat{\alpha}, \quad (4.48)$$

where $O(\hat{\alpha}, \hat{\gamma})$ denotes the two dimensional Fourier transform of the object function. Denoting $U_s(\omega, d)$ as the Fourier transform of the scattered field along the receiver array with respect to x such that

$$U_s(\omega, d) = \int u_s(x, d) \exp[-i\omega x] dx. \quad (4.49)$$

Now, substituting Eq. (4.48) into Eq. (4.49) and noting that

$$\int_{-\infty}^{\infty} \exp[i(\omega - a)x] dx = 2\pi\delta(\omega - a), \quad (4.50)$$

where $\delta(\omega)$ is the Dirac delta function, yields

$$U_s(\hat{\alpha}, d) = \frac{i}{2\sqrt{k_0^2 - \hat{\alpha}^2}} O(\hat{\alpha}, \sqrt{k_0^2 - \hat{\alpha}^2} - k_0) \exp[i(\sqrt{k_0^2 - \hat{\alpha}^2} - k_0)d]. \quad (4.51)$$

Equation (4.51) defines the Fourier Diffraction Theorem stated previously. It can be seen that the factor

$$\frac{i\pi}{\sqrt{k_0^2 - \hat{\alpha}^2}} \exp[i(\sqrt{k_0^2 - \hat{\alpha}^2} - k_0)d],$$

is simply a constant for a given measurement line. When $\hat{\alpha}$ varies from $-k_0$ to k_0 the coordinates $(\hat{\alpha}, \sqrt{k_0^2 - \hat{\alpha}^2} - k_0)$ trace out a semicircular arc in the (u, v) plane as shown in Fig. 4.21.

A similar derivation can be performed to extend the Fourier Diffraction Theorem to three dimensions as outlined in (Wang et al. 2004).

Interpolation

Given the scattered field from a single projection angle, we may determine the spatial Fourier transform of the object function along an arc. However, this alone is not sufficient to determine an accurate estimate of the object function of the target. By rotating

4.5 T-ray Diffraction Tomography

the target we obtain the scattered field at different orientations. Each of these provide an estimate of the spatial Fourier transform of the object function along a different arc. The arcs rotate as the target is rotated (Mueller et al. 1980), and by rotating through 360° the full Fourier space may be populated, up to a maximum spatial frequency of $\sqrt{2}k$, where $k = 2\pi/\lambda$ is the propagation number of the incident field. This process is illustrated in Fig. 4.23.

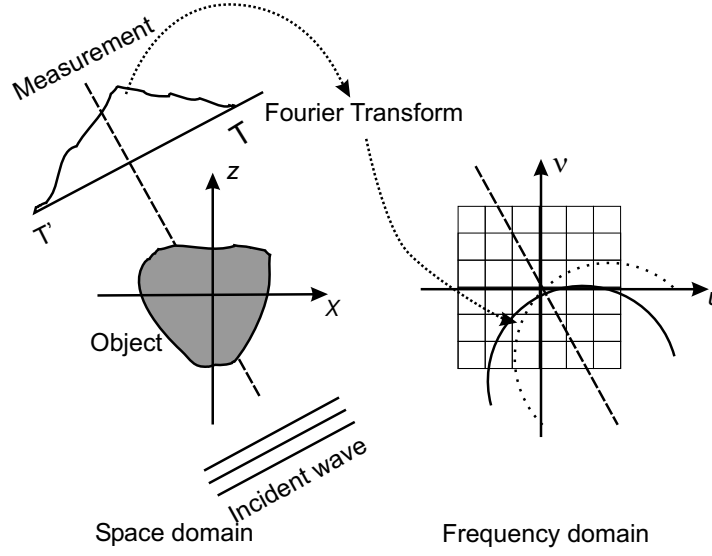


Figure 4.23. Illustration of interpolation for diffraction tomography. By rotating the target, O may be estimated on different semicircular arcs each oriented at the same angle θ as the wave vector. In this way the spatial Fourier domain may be populated and interpolation is used to determine the values of O on a rectangular grid.

To reconstruct the target we hope to apply the 2D inverse Fourier transform, which requires the data to be estimated on a regular grid. There are two common methods of estimating the Fourier coefficients on a grid based on the semicircular arc data. These are by performing interpolation in either the space or the frequency domain. Interpolation in the space domain allows the mathematically elegant method of *filtered backpropagation* to be used (Devaney 1982, Kaveh et al. 1982). However this method is computationally more demanding than frequency domain interpolation without providing any accuracy advantage. In this Thesis bilinear interpolation was performed in the frequency domain.

Before interpolation can be performed it is necessary to translate the arc coordinates $(\hat{a}, \sqrt{k_0^2 - \hat{a}^2} - k_0)$, oriented at the projection angle θ , to cartesian coordinates (u, v) . The derivation of the translation formula is performed by translating first to standard

polar coordinates and then to cartesian coordinates (Pan and Kak 1983). The results are

$$\begin{aligned}\hat{\alpha} &= k \sin \left\{ 2 \sin^{-1} \left(\frac{\sqrt{u^2 + v^2}}{2k} \right) \right\}, \quad \text{and} \\ \theta &= \tan^{-1} \left(\frac{v}{u} \right) + \sin^{-1} \left(\frac{\sqrt{u^2 + v^2}}{2k} \right) + \frac{\pi}{2}.\end{aligned}\quad (4.52)$$

Therefore, to convert each point on a rectangular grid to the $(\hat{\alpha}, \theta)$ domain, the desired (u, v) values are substituted into Eq. (4.52). This does not necessarily result in values of $(\hat{\alpha}, \theta)$ for which O is known. In this case bilinear interpolation of the closest known values is used. Mathematically, O is known on $N_{\hat{\alpha}} \times N_{\theta}$ uniformly spaced samples with sampling intervals of $\Delta\hat{\alpha}$ and $\Delta\theta$ in the $\hat{\alpha}$ and θ axes respectively. Given values of $(\hat{\alpha}$ and $\Delta\theta)$ for which O is required to be estimated, the estimate is given by

$$O(\hat{\alpha}, \theta) = \sum_{i=1}^{N_{\hat{\alpha}}} \sum_{j=1}^{N_{\theta}} O(\hat{\alpha}_i, \theta_j) h_1(\hat{\alpha} - \hat{\alpha}_i) h_2(\theta - \theta_j), \quad (4.53)$$

where

$$h_1(\hat{\alpha}) = \begin{cases} 1 - \frac{|\hat{\alpha}|}{\Delta\hat{\alpha}} & |\hat{\alpha}| \leq \Delta\hat{\alpha} \\ 0 & \text{otherwise} \end{cases}, \quad (4.54)$$

$$h_2(\theta) = \begin{cases} 1 - \frac{|\theta|}{\Delta\theta} & |\theta| \leq \Delta\theta \\ 0 & \text{otherwise} \end{cases}. \quad (4.55)$$

Once O is computed on a regular grid the 2D inverse Fast Fourier transform (FFT) is used to recover the object function $o(x, y)$.

4.5.4 Experimental Results

Born Approximation

These diffraction tomography methods are only applicable to weakly scattering objects so the test targets were restricted to plastic materials with low refractive index (< 1.5). In the future non-linear iterative techniques will enable more general targets to be reconstructed.

4.5 T-ray Diffraction Tomography

To test the T-ray diffraction tomography system, a sample was designed such that the Born approximation was valid. A small solid vertical cylinder of high density polyethylene (HDPE) cylinder was used. HDPE has a refractive index of 1.5 at THz frequencies and is relatively dispersionless over the frequency range 0.1 – 10 THz. The diameter of the cylinder was 1 mm. The condition for the validity of the Born approximation is given in Eq. (4.34). For this sample $a = 1$ mm, and $n_\delta = 0.5$. The inequality in Equation (4.34) becomes $\lambda > 2$ mm. Therefore the Born approximation is valid for this target for frequencies under 150 GHz.

The target was placed 48 mm from the ZnTe detector in Fig. 4.20 and imaged over 100 temporal steps and 36 projection angles. The geometry of the experiment is illustrated in Fig. 4.24. To improve the SNR, 100 frames were averaged for each sample. The measured time domain pulses were Fourier transformed and the complex amplitude at a frequency of 100 GHz was used for the reconstruction. The sample was then removed and the THz response measured without the sample to provide a measurement of u_0 . The scattered field $u_s(\mathbf{r})$ was estimated by subtracting u_0 from the total measured field according to Eq. (4.24). Figure 4.25 shows the calculated $u_s(\mathbf{r})$ image at a single projection angle and at a frequency of 0.1 THz. The effects of diffraction around the cylinder's body are clearly visible. The data was averaged in the vertical dimension and the 2D reconstruction algorithm described in Sec. 4.5.3 was employed based on the first Born approximation. This approximation is only valid for small targets but was able to reconstruct the cross-section of this simple target as shown in Fig. 4.26 (Ferguson et al. 2002c).

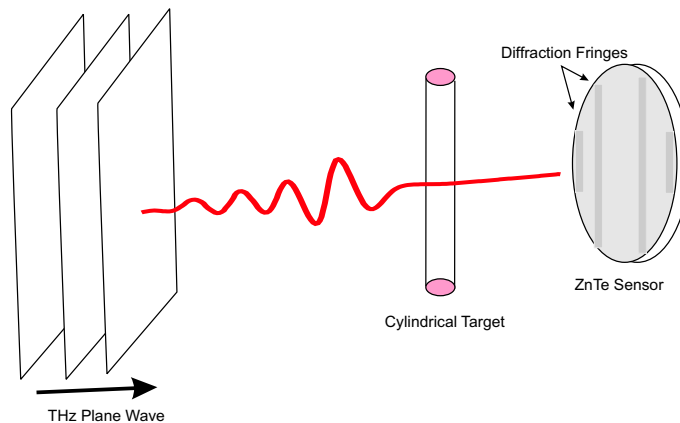


Figure 4.24. The geometry of the T-ray DT experiment. A thin vertical cylinder is illuminated with a quasi-plane wave THz beam. The radiation diffracted by the target is measured on a ZnTe sensor and detected using a CCD (not shown).

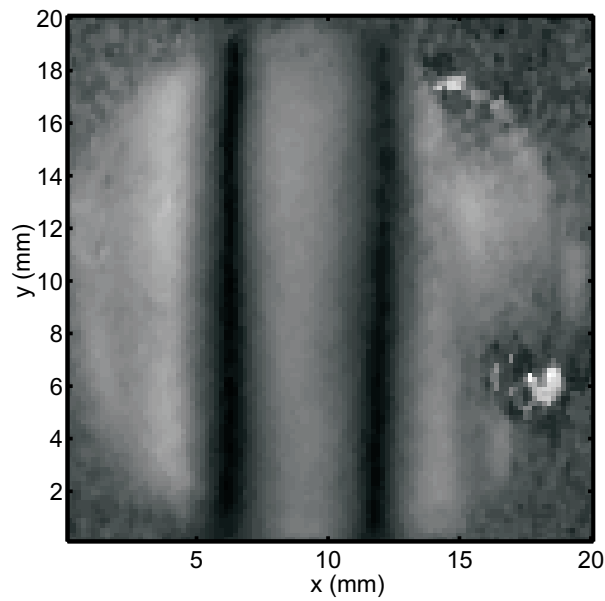


Figure 4.25. THz image of a thin polyethylene cylinder for a single projection angle. The measured data was used to calculate $u_s(\mathbf{r})$, this was Fourier transformed and the amplitude at a frequency of 0.1 THz is plotted. The 2 cm diameter circular aperture of the detector is visible as are two vertical lines resulting from diffraction of the THz radiation.

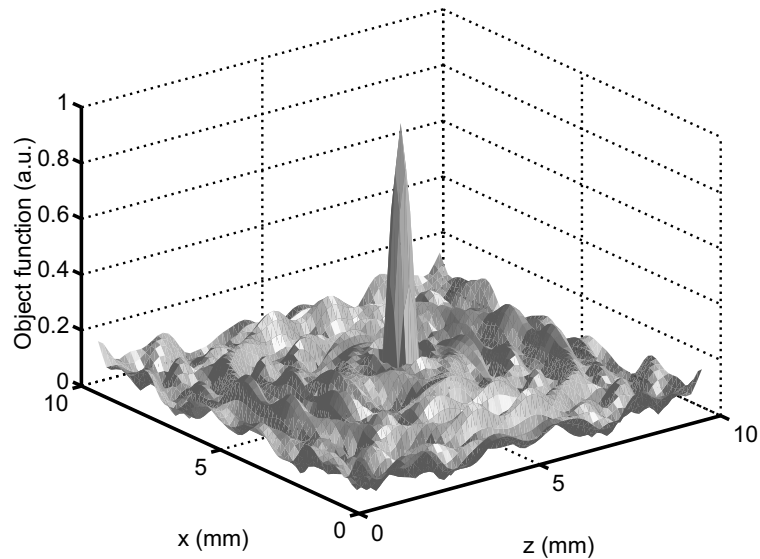


Figure 4.26. Reconstructed cross-section of the polyethylene cylinder. The Fourier Diffraction Theorem was used to allow the cross-section of the cylinder to be reconstructed. The reconstruction was based on the first Born approximation to the wave equation. The height of the figure shows the intensity of the reconstructed object function and is related to the refractive index.

4.5 T-ray Diffraction Tomography

The reconstruction shown in Fig. 4.26 shows that the reconstructed object function tapers to a tip. This is a result of the low pass filtering operation implicit in the Fourier Diffraction Theorem. Only spatial frequency components less than $\sqrt{2}k$ are recovered. This results in blurring of sharp edges in the reconstructed image. The resolution of the reconstruction is of the order of the wavelength λ . The filtering is less severe as the frequency used for the reconstruction, and hence k , are increased. However, at higher frequencies the Born approximation is no longer valid and accurate reconstructions were not possible. For this reason the Rytov approximation is favoured for T-ray DT.

Rytov Approximation

A more complicated sample was constructed to investigate the properties of the system with a Rytov approximation based reconstruction algorithm. The target structure consisted of 3 rectangular polyethylene cylinders. This test structure is illustrated in Fig. 4.27 and the geometry shown in Fig. 4.28.



Figure 4.27. A test structure imaged by the T-ray DT system. The target consisted of 3 rectangular polyethylene cylinders.

The cylinders were made larger than the previous example in order to test the limits of the reconstruction algorithm. The cylinder dimensions were beyond the valid range for the Born approximation and hence the Rytov approximation was adopted.

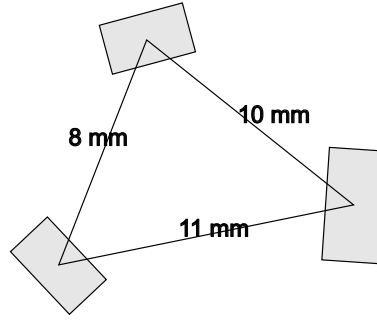


Figure 4.28. The geometry of the T-ray DT test structure. The rectangular cylinders shown in Fig. 4.27 had dimensions of 2.0×1.5 , 3.5×1.5 and 2.5×1.5 mm (clockwise from top).

The target was again imaged at 100 temporal steps and 36 projection angles. While the input for the Born approximation based reconstruction is simply the total measured field minus the measured incident field, the Rytov approximation requires a slightly more involved calculation. As discussed in Sec. 4.5.3 the Fourier Diffraction Theorem for the Born approximation is expressed in terms of the scattered field $u_s(\mathbf{r})$. The analogous quantity for the Rytov based reconstruction is $\phi_s(\mathbf{r})u_0$. To apply the Rytov based reconstruction we need to determine $\phi_s(\mathbf{r})$ from the measured $u_s(\mathbf{r})$ and u_0 . This is done by recalling that

$$u(\mathbf{r}) = u_0 + u_s(\mathbf{r}) = e^{\phi_0 + \phi_s(\mathbf{r})}, \quad (4.56)$$

rearranging we find that

$$\begin{aligned} u_s(\mathbf{r}) &= e^{\phi_0 + \phi_s(\mathbf{r})} - e^{\phi_0}, \\ &= e^{\phi_0} (e^{\phi_s(\mathbf{r})} - 1), \\ &= u_0 (e^{\phi_s(\mathbf{r})} - 1). \end{aligned} \quad (4.57)$$

Inverting this expression gives

$$\phi_s(\mathbf{r}) = \ln \left[\frac{u_s(\mathbf{r})}{u_0} + 1 \right]. \quad (4.58)$$

This allows the quantity, $\phi_s(\mathbf{r})u_0$, to be estimated from the measured diffraction data and allows a Rytov based reconstruction to be performed. The results of the reconstruction for the target shown in Fig. 4.27 are shown in Fig. 4.29. The 2D reconstruction was performed using a frequency of 0.3 THz, which provided the maximum SNR for the antenna THz source. The scattered fields at each height were averaged to provide a high fidelity reconstruction.

4.5 T-ray Diffraction Tomography

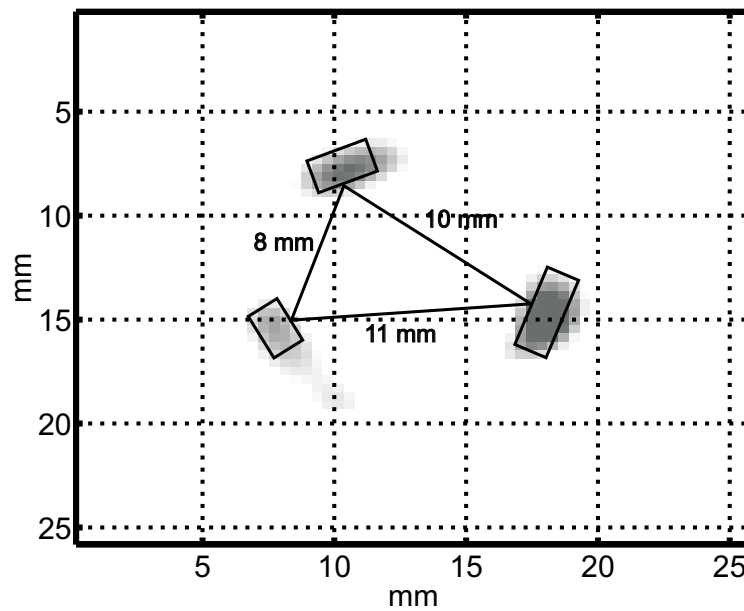


Figure 4.29. Reconstructed cross-section of the polyethylene cylinders. The reconstructed object function was thresholded at 50% of the peak amplitude. This provided an accurate reconstruction of the three cylinders. The actual geometry of the cylinders is overlaid on the figure.

The previous reconstructions demonstrate the reconstruction of a target's 2D (x, z) cross-section. The reconstruction algorithm described in Sec. 4.5.3 is general and extends to 3 dimensions (Wolf 1969). Typical diffraction tomography methods use an array of detectors, which restricts them to 2D reconstructions. However, because the T-ray DT system uses a CCD to capture the scattered field over a 2D planar array, full 3D reconstructions are possible. Experimentally the 3D reconstruction is substantially more difficult. For a 2D reconstruction the vertical CCD pixels were averaged to improve the SNR, additionally the small size of the ZnTe sensor implies that the scattered field is only measured over a limited range and is assumed to be zero outside this range. This introduces errors in the reconstruction. This problem is highlighted in Fig. 4.30 where the scattered phase is plotted as a function of x . The assumption that the phase beyond the sensor is zero is clearly inaccurate.

For these reasons an alternate method (termed T-ray Computed Tomography) was devised to allow 3D reconstructions to be performed (see Sec. 4.6). For certain targets, provided the variation in the y -axis is not too severe, a quasi-3D reconstruction may be performed by performing a 2D reconstruction on each horizontal slice of the measured CCD data. The reconstructed slices may then be combined to form a 3D image. This

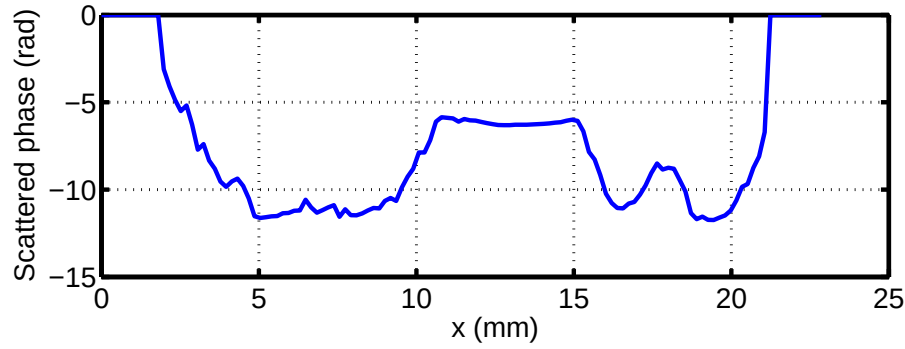


Figure 4.30. Phase of the scattered field $\phi_s(r)$ measured across the CCD. The phase of the scattered field was calculated based on the measured diffraction data and is plotted for a single projection angle. The phase outside the measured range is assumed to be zero. Because the sensor crystal only captures the scattered field over a small range this results in errors in the reconstruction. This plot highlights the fact that the scattered phase beyond the sensor is unlikely to be zero in practice.

was performed for the target shown in Fig. 4.27 and is illustrated in Fig. 4.31. Each reconstructed slice was thresholded at 50% of the peak amplitude, the slices were then combined and surface rendered to generate a 3D image.

T-ray diffraction tomography reconstructs the target's object function, which is related to its refractive index by Eq. (4.23). This equation may be inverted to determine the refractive index of the target. This was performed and the refractive index profile of the three cylinders is shown in Fig. 4.32. The HDPE cylinders have a THz refractive index of 1.5 while the reconstructed value is approximately 1.3. There are two reasons for this discrepancy. The first follows from the problem of the limited size of the detector as discussed above. As a result not all the scattered field is measured and this results in low pass filtering of the reconstructed image (Natterer and Wübbeling 2001). The second problem is caused by the small size of the target and the spatial resolution of the Fourier Diffraction Theorem. The Fourier Diffraction Theorem only allows spatial frequency components up to $\sqrt{2}k$ to be reconstructed. This results in a low pass filtering of the reconstructed target. In the example considered here, these two low pass filtering effects act to smear out the reconstructed cylinders and as a result reduce the peak reconstructed refractive index. This effect could be alleviated by either moving to a higher frequency, or increasing the size of the sensor crystal relative to the target size.

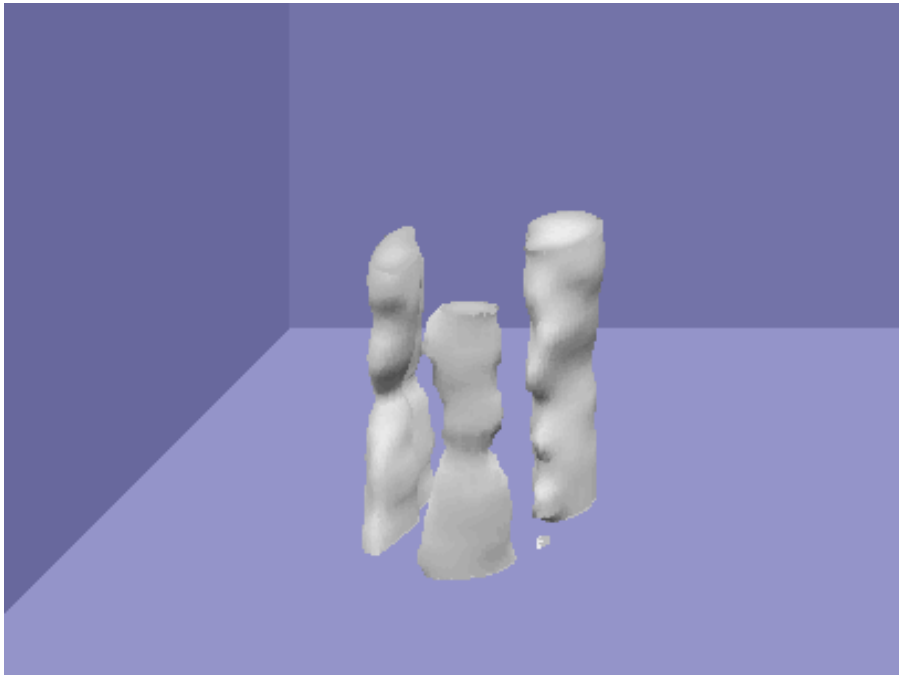


Figure 4.31. Reconstructed 3D image of the polyethylene cylinders. Each horizontal slice was reconstructed independently and combined to form a 3D image. The reconstructions were thresholded at 50% of the peak amplitude and surface rendered. The visible ripples on the surface of the cylinders are a result of the thresholding procedure and are caused by noise in the reconstructions.

T-ray diffraction tomography allows the reconstruction to be performed at multiple frequencies to allow spectroscopic information to be inferred. The prototype system demonstrated in this Thesis used a planar stripline antenna to provide high peak THz power. This source generates low bandwidth THz radiation with a peak frequency around 0.2 THz. The reconstruction may be performed at higher frequencies, however, the THz power and thereby the SNR decrease as the frequency increases. Thus, while higher frequency reconstructions theoretically result in higher fidelity images, in practice the artifacts introduced by lower SNR result in significant degradation of the results. This is illustrated in Fig. 4.33 where the target shown in Fig. 4.27 was reconstructed using the T-ray DT data at 0.2 THz, 0.3 THz and 0.4 THz. As the frequency increases the reconstructed peak refractive index of the cylinders approach the true value of 1.5, however the images are degraded by increased noise in the measurements.

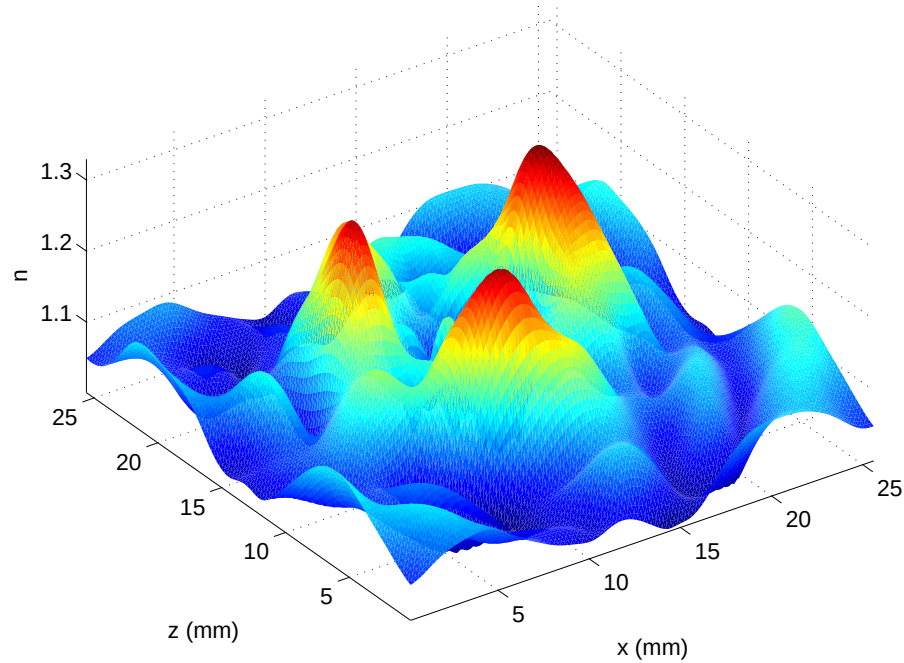


Figure 4.32. Reconstructed refractive index of the polyethylene cylinders. The three cylinders are clearly differentiated, however the image is low pass filtered as a result of the reconstruction algorithm. The cylinders are clearly smeared out as a result.

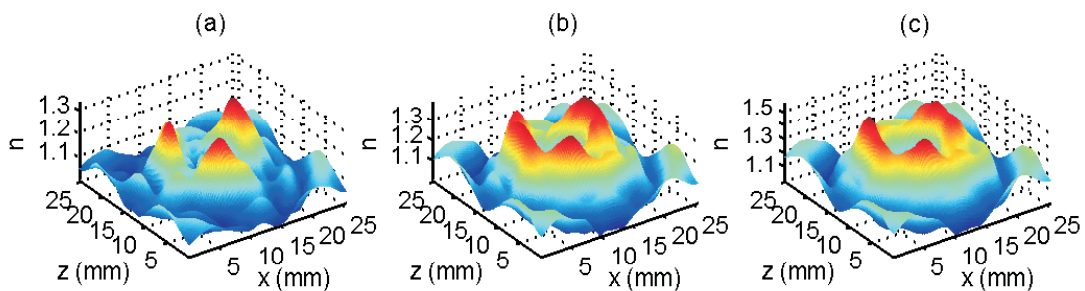


Figure 4.33. T-ray DT reconstruction performed at 3 different frequencies. The target shown in Fig. 4.27 was reconstructed using the T-ray DT data at three frequencies: (a) 0.2 THz, (b) 0.3 THz and (c) 0.4 THz.

4.5.5 Summary

T-ray diffraction tomography builds on existing methods of linearised inverse scattering by applying the well-established reconstruction algorithms to the THz frequency range. It demonstrates that the approximations employed remain valid at high frequencies and, through the use of 2D FSEOS imaging allows tomographic images to be reconstructed without requiring multiple detectors. This section has demonstrated the limitations of the Born and Rytov approximations and highlighted the spatial low pass filtering effects inherent in the Fourier Diffraction Theorem based reconstruction.

The reconstruction is hindered by the relatively low SNR of the THz field measurements. More advanced algorithms are available for reconstructing the T-ray DT data including the MGF and CSI algorithms (Kleinman and van der Berg 1992, van den Berg and Kleinman 1997). These will allow a wider range of targets to be reconstructed but convergence is not guaranteed and they are likely to struggle with the amount of noise given the current system. Time domain algorithms for diffraction tomography (Mast 1999, Melamed et al. 1996) have shown improved image quality over the frequency domain methods considered here. However these methods assume that the target is dispersionless, which removes a key advantage of THz techniques, that of spectroscopic information extraction.

4.6 T-ray Computed Tomography

4.6.1 Introduction

The most well known and successful transmission tomography technology is X-ray Computed Tomography. Developed in the early 1970s, X-ray CT systems have had a remarkable impact on modern medicine. The linearised inverse scattering methods discussed in Sec. 4.5 perform well, however they impose severe restrictions on the size and contrast of the target and with the current technology suffer from severe SNR problems. T-ray computed tomography seeks to emulate the success of X-ray CT by considering the algorithms and techniques used in this field and adapting them to THz imaging systems.

4.6.2 X-ray Tomography

Background

X-ray Computed Tomography (CT) imaging is also known as ‘CAT scanning’ (Computed Axial Tomography). The modern form of X-ray CT was developed in 1972 by British engineer Godfrey Hounsfield of EMI Laboratories, England (Hounsfield 1973), based on theoretical work performed by South African born physicist Allan Cormack at Tufts University, Massachusetts (Cormack 1963, Cormack 1964). The pair shared the 1979 Nobel Prize for Medicine for their contribution, which ultimately revolutionised medical imaging.

The first clinical CT scanners were installed between 1974 and 1976. They became widely available by about 1980, and they are now ubiquitous with over 30,000 installed worldwide (Jones and Singh 1993).

An excerpt from Cormack and Hounsfield’s Nobel Prize citation reads,

‘It is no exaggeration to state that no other method with X-ray diagnostics within such a short period of time has led to such remarkable advances in research and in a multiple of applications as computer assisted tomography.’

Mathematics

X-ray CT reconstruction algorithms are based on the *Radon Transform*. The most popular of these reconstruction methods is known as *filtered backprojection* and these concepts are detailed in this section.

In X-ray CT the attenuation of X-rays along their propagation path through an object can be expressed as a line integral of the absorption coefficient of the object along a line (Herman 1980). The following equation expresses this relation:

$$p(\theta, l) = \int_{L(\theta, l)} o(x, z) dl = \Re \{o(x, z)\}, \quad (4.59)$$

where $p(\theta, l)$ is termed the projection and is a function of the projection angle θ , and the distance from the axis of rotation perpendicular to the ray propagation, l . The variable $o(x, y)$ is the object function of the target. The integral is calculated over the straight line L joining the source and the detector. This transformation is known as the Radon transform and is denoted $\Re$. This basic concept is depicted in Fig. 4.34.

Explicit inversion algorithms for the Radon transform were derived as early as 1917 (Radon 1917), however, these methods were only applicable in 2 dimensions and were not physically useful as they required knowledge of all possible projections and were overly sensitive to noise in the measurements (Natterer 1986). Nevertheless Radon's contribution was a significant one and his derivation is presented in Appendix D in honour of its historical significance. Cormack and Hounsfield developed practical reconstruction algorithms that allowed physical X-ray tomography systems to be developed. Today the most commonly employed reconstruction technique is the filtered backprojection algorithm, which was first developed independently by Bracewell and Riddle (1967) and Ramachandran and Lakshminarayanan (1971) and later advanced by Shepp and Logan (1974). The following derivation follows that outlined in Kak and Slaney (2001).

Denoting the Fourier transform of $p(\theta, l)$ with respect to l as $P(\theta, \nu)$, the Fourier transformation of Eq. (4.59) is,

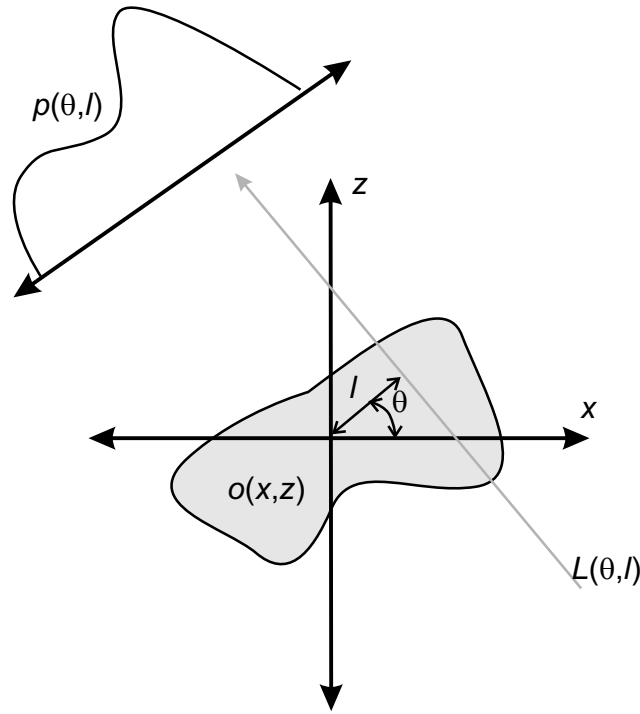


Figure 4.34. An object, $o(x, z)$, and its projection, $p(\theta, l)$. The Radon transform defines the projection $p(\theta, l)$ as the line integral over the straight line L of the object function $o(x, z)$. The projection offset, l , is the perpendicular distance of the projection from the axis of rotation. Here, θ defines the projection angle and x and z define a standard rectangular coordinate system.

$$\begin{aligned}
 P(\theta, \nu) &= \int_{-\infty}^{+\infty} p(\theta, l) \exp(-i\nu l) dl, \\
 &= \int_{-\infty}^{+\infty} dl \iint_{-\infty}^{+\infty} \delta(x \sin(\theta) - z \cos(\theta) - l) o(x, z) \exp(-i\nu l) dx dz, \\
 &= \iint_{-\infty}^{+\infty} \exp[-i\nu(x \sin(\theta) - z \cos(\theta))] o(x, z) dx dz, \\
 &= \iint_{-\infty}^{+\infty} \exp[-i(\eta x - \xi z)] o(x, z) dx dz,
 \end{aligned} \tag{4.60}$$

where $\nu = 2\pi/l$ is the spatial frequency along the l axis and $\eta = \nu \sin(\theta)$ and $\xi = \nu \cos(\theta)$. The right hand side of Equation (4.60) can be seen to be the 2D spatial Fourier transform of the object function, where $\eta = \nu \sin(\theta)$ and $\xi = \nu \cos(\theta)$ are the spatial frequency component along the x and z directions, respectively. This result is known as the *Fourier Slice Theorem* and is a limiting case of the Fourier Diffraction Theorem

4.6 T-ray Computed Tomography

discussed in Sec. 4.5.3. Here, $p(\theta, l)$ can be obtained by measuring the signal at various θ and l via rotating, and translating either the source and detector or the target. In this way the object function in the spatial (x, z) domain is mapped to the (θ, l) domain.

To reconstruct the target's object function $o(x, z)$ the *filtered backprojection* algorithm is used. The starting point for the derivation of the filtered backprojection algorithm is the inverse Fourier transform of the object function,

$$o(x, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} O(\xi, \eta) \exp(i2\pi(\xi x + \eta z)) d\xi d\eta. \quad (4.61)$$

To change variables from the rectangular coordinate system (ξ, η) to a polar coordinate system (ν, θ) the following substitutions are made

$$\xi = \nu \cos \theta, \quad (4.62)$$

$$\eta = \nu \sin \theta, \quad (4.63)$$

$$d\xi d\eta = \nu d\nu d\theta, \quad (4.64)$$

whereby

$$o(x, z) = \int_0^{2\pi} \int_0^{\infty} O(\nu, \theta) \exp[i2\pi\nu(x \cos \theta + z \sin \theta)] \nu d\nu d\theta. \quad (4.65)$$

By observing that in polar coordinates $O(\nu, \theta + \pi) = O(-\nu, \theta)$ the integral from 0 to 2π can be reduced to 0 to π by simply replacing the term ν by $|\nu|$ and performing the second integral from $-\infty$ to ∞ . Additionally, setting $l = x \cos \theta + z \sin \theta$ yields

$$o(x, z) = \int_0^{\pi} \left\{ \int_{-\infty}^{\infty} O(\nu, \theta) |\nu| \exp[i2\pi\nu l] d\nu \right\} d\theta. \quad (4.66)$$

Using the Fourier Slice Theorem Eq. (4.60) we obtain the equation that defines the filtered backprojection algorithm:

$$o(x, z) = \int_0^{\pi} \left\{ \int_{-\infty}^{\infty} P(\theta, \nu) |\nu| \exp[2\pi i \nu l] d\nu \right\} d\theta. \quad (4.67)$$

To illustrate how the filtered backprojection algorithm is typically implemented it may be expressed as

$$o(x, z) = \int_0^{\pi} q_{\theta}(x \cos \theta + z \sin \theta) d\theta, \quad (4.68)$$

where

$$q_{\theta}(l) = \int_{-\infty}^{\infty} P_{\theta}(\nu) |\nu| \exp(i2\pi\nu l) d\nu. \quad (4.69)$$

Equation (4.69) can be seen as a filtering operation. The function $p_\theta(l)$ is termed the projection for a given projection angle θ . The *filtered projection* $q_\theta(l)$ is calculated by Fourier transforming $p_\theta(l)$, filtering the result using a filter with a frequency response of $|\nu|$ and then inverse Fourier transforming the result. The filter $|\nu|$ is known as the *Ram-Lak* filter, it serves as a type of high pass filter and amplifies the high spatial frequency components of the projection. In practice other filters such as Hamming or Hanning windows (Hamming 1977) may be also applied to reduce the noise amplification inherent in the Ram-Lak filter. The filtered backprojection algorithm, Eq. (4.68), allows the object function at each value of (x, z) to be reconstructed. For a point (x, z) there is a corresponding value of $l = x \cos \theta + z \sin \theta$ for each projection θ . The value of $o(x, z)$ is recovered by summing the value of the filtered projections at the corresponding l over all angles θ . In the discrete case l may not always be known at the required value and in this case bilinear interpolation is most often used and produces highly accurate results.

4.6.3 T-ray CT Reconstruction Algorithm

“All models are wrong, some are useful.”

- G. E. P. Box (Box 1976)

The Radon transform was derived for X-ray propagation, where the extremely short wavelength and high energy of X-ray photons reduce diffraction effects to the point where geometric approximations are valid. As seen earlier in this Chapter, T-ray propagation is strongly influenced by diffraction effects and a straight-line propagation model is not valid in the general case.

To attempt to use inverse Radon transform methods for the inversion of THz frequency radiation at first glance appears quite naïve. X-ray photons have an energy over 10^7 times that of T-ray photons, similarly X-ray radiation has a wavelength of the order of $1 \text{ \AA}$ (10^{-10} m), compared to 0.3 mm at 1 THz . While the line-integral based Radon transform is accepted as a reasonably accurate model of X-ray absorption through media such as the human body, it is well known that in general it cannot be used to describe the propagation of lower frequency radiation, such as optical, terahertz or RF radiation. It is obvious then, that the use of the Radon transform for THz tomography requires substantial innovation and justification.

4.6 T-ray Computed Tomography

This section provides a mathematical derivation justifying the use of inverse Radon transform methods for T-ray tomography, via the unique concept of *coherent* tomography. In the process, it derives a number of optical design guidelines that must be met for the reconstruction algorithm to be valid. This allows the use of extremely efficient and relatively simple reconstruction algorithms, which stands in stark contrast to the methods typically employed in the neighbouring frequency bands on either side. Complex iterative methods are used to invert the Helmholtz equation Eq. (4.22) in the RF band and the diffusion equation Eq. (4.3) in the NIR and optical bands.

An important parameter to the following discussion is that of the Rayleigh range, z_0 . For a Gaussian beam the Rayleigh range is used to describe the beam propagation. If z is the optical axis of the beam and $z = 0$ defines the focal plane, then the minimum beam waist W_0 is given by

$$W_0 = \sqrt{\frac{\lambda z_0}{\pi}}, \quad (4.70)$$

and the beam radius $W(z)$, as a function of z is given by

$$W(z) = W_0 \sqrt{1 + \left(\frac{z}{z_0}\right)^2}. \quad (4.71)$$

The depth of focus of the beam is defined as twice the Rayleigh range as illustrated in Fig. 4.35.

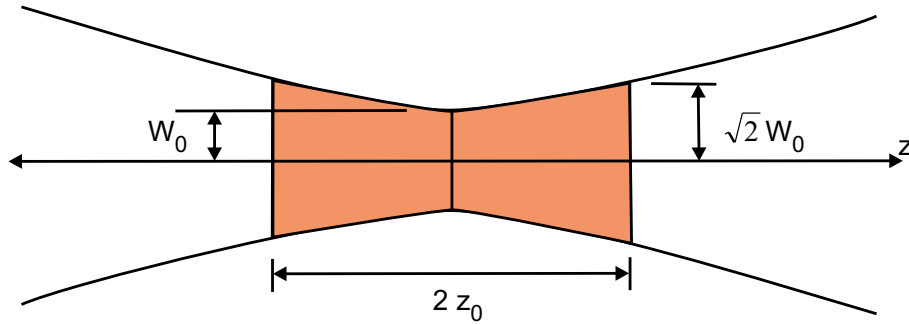


Figure 4.35. The depth of focus of a Gaussian beam. A Gaussian beam has a minimum beam waist of W_0 at its focus. Beyond the focus the beam expands. The range over which the beam radius is less than $\sqrt{2}W_0$ is referred to as the depth of focus. It is equal to twice the Rayleigh range, z_0 . After (Saleh and Teich 1991).

The following analysis follows that presented in Wang et al. (2004). It shows that it is possible to design a THz system such that a Radon transform based propagation model is satisfied by focusing the THz beam on the target (rather than broad beam illumination as in diffraction tomography) and making the following two assumptions:

1. The target's lateral extent in the direction of the THz wave vector is less than the Rayleigh range of the THz beam.
2. Within the Rayleigh range the THz beam propagates as a planar Gaussian wave.

Under these two assumptions THz propagation can be shown to comply with a Radon transform based model. The derivation commences with the Rytov approximation to the wave equation described in Sec. 4.5.1. Given the same definitions of the total, incident and scattered fields from Sec. 4.5.1:

$$u(\mathbf{r}) = e^{\phi_0(\mathbf{r}) + \phi_s(\mathbf{r})} = u_0(\mathbf{r}) \exp[\phi_s(\mathbf{r})], \quad (4.72)$$

where the incident field is directed along the z -axis such that

$$u_0(\mathbf{r}) = \exp(ik_0 z). \quad (4.73)$$

It can be shown (Born and Wolf 1999) that

$$\begin{aligned} \phi_s(\mathbf{r}) &= \frac{1}{u_0(\mathbf{r})} \int G(\mathbf{r} - \mathbf{r}') o(\mathbf{r}') u_0(\mathbf{r}') d\mathbf{r}' \\ &= \frac{1}{4\pi} \int_V \frac{\exp(ik_0 |\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} o(\mathbf{r}') \times \exp[-ik_0 \hat{\mathbf{z}} \cdot (\mathbf{r} - \mathbf{r}')] d\mathbf{r}', \end{aligned} \quad (4.74)$$

where, as defined previously, $\phi_s(\mathbf{r})$ is the complex phase of the scattered field at position $\mathbf{r}$, $u_0(\mathbf{r})$ is the incident field, k_0 is the propagation number of the incident radiation in a vacuum, $G(\mathbf{r} - \mathbf{r}')$ is the Green's function, $\hat{\mathbf{z}}$ is a unit vector along the z -axis, $o(\mathbf{r})$ is the object function of the target and V is a volume encompassing the target.

The complex phase on the measurement plane ($z = d$) defined in Fig. 4.22 is given by (Gbur and Wolf 2001)

$$\begin{aligned} \phi_s(x, y, d) &= \frac{i}{8\pi^2} \int_V o(\mathbf{r}') d\mathbf{r}' \iint \frac{1}{\hat{\gamma}} \exp[i(\hat{\gamma} - k_0)(d - z')] \\ &\quad \times \exp[i\hat{\alpha}(x - x') + i\hat{\beta}(y - y')] d\hat{\alpha} d\hat{\beta} \end{aligned} \quad (4.75)$$

where d is the distance from the origin to the measurement plane, $(\hat{\gamma}, \hat{\alpha}, \hat{\beta})$ are vector coefficients of a Weyl spherical wave in the (z, x, y) directions such that the $(\hat{\alpha}, \hat{\beta})$ plane defines the measurement plane and $\hat{\gamma} = \sqrt{k_0^2 - \hat{\alpha}^2 - \hat{\beta}^2}$.

Under the two assumptions described above, the resultant field propagation wavevector does not deviate significantly and $\hat{\alpha} = \hat{\beta} \approx 0$ and $\hat{\gamma} \approx k_0$. The term $\exp[i(\hat{\gamma} -$

4.6 T-ray Computed Tomography

$k_0)(d - z')]$ in Eq. (4.74) can then be expanded in a Taylor series about $\hat{\alpha} = \hat{\beta} = 0$ such that

$$\begin{aligned} & \exp[i(\hat{\gamma} - k_0)(d - z')] \\ \approx & 1 - \frac{\hat{\alpha}^2 + \hat{\beta}^2}{2k_0}(d - z')i + \mathbb{O}[(\hat{\alpha}^2 + \hat{\beta}^2)^2] + \dots, \end{aligned} \quad (4.76)$$

where $\mathbb{O}(x)$ denotes a term of order x . When the second term is much smaller than 1, the first term will dominate and the other terms may be safely discarded. The conditions for this approximation are investigated in Sec. 4.6.4. Using the first term, Eq. (4.74) can be further simplified as (Gbur and Wolf 2001)

$$\phi_s(x, y, d) = \frac{i}{8\pi^2} \int_V o(\mathbf{r}') d\mathbf{r}' \iint \frac{1}{\hat{\gamma}} \exp[i\hat{\alpha}(x - x') + \hat{\beta}(y - y')] d\hat{\alpha} d\hat{\beta}. \quad (4.77)$$

The $\hat{\alpha}, \hat{\beta}$ integration can be evaluated using the Fourier representation of the Dirac delta function,

$$\iint \exp[i\hat{\alpha}(x - x') + \hat{\beta}(y - y')] d\hat{\alpha} d\hat{\beta} = (2\pi)^2 \delta(x - x') \delta(y - y'). \quad (4.78)$$

Inserting Eq. (4.78) into Eq. (4.77) and using k_0 to replace $\hat{\gamma}$, yields

$$\phi_s(x, y, d) = \frac{i}{2k_0} \int_V o(\mathbf{r}') \delta(x - x') \delta(y - y') d\mathbf{r}'. \quad (4.79)$$

Therefore, the measured phase term at a sensor positioned at $z = d$ can be written

$$\phi_s(x, y, d) = \frac{i}{2k_0} \int_V o(x, y, z') dz'. \quad (4.80)$$

Recalling $o(x, y, z') = k_0^2 [\tilde{n}(\omega, x, y, z')^2 - 1]$, the scattered phase is

$$\phi_s(x, y, d) = \frac{i}{2k_0} \int_L k_0^2 [\tilde{n}(\omega, x, y, z')^2 - 1] dz', \quad (4.81)$$

where L is the line over which the THz field propagates through the target.

When $n \approx 1$, then the refractive index deviation $\tilde{n}_\delta(\omega, \mathbf{r}) = \tilde{n}(\omega, \mathbf{r}) - 1$ is small and the term $\tilde{n}(\omega, x, y, z')^2 - 1$ can be approximated

$$\tilde{n}(\omega, x, y, z')^2 - 1 \approx 2\tilde{n}_\delta(\omega, \mathbf{r}). \quad (4.82)$$

Combining Eq. (4.82), Eq. (4.81) and Eq. (4.72), reveals (Ferguson et al. 2002b, Wang et al. 2004)

$$u(x, y, d) = u_0(x, y, d) \exp \left[ik_0 \int_L \tilde{n}_\delta(\omega, \mathbf{r}) dz' \right]. \quad (4.83)$$

The total complex phase change of the scattered THz field can therefore be approximately described by a line integral of the complex refractive index of the target. This equation is of the same form as Eq. (4.59) and the filtered backprojection algorithm can be applied to reconstruct $\tilde{n}_\delta(\omega, \mathbf{r})$. The complex refractive index is given by

$$\begin{aligned}\tilde{n}(\omega, \mathbf{r}) &= n(\omega, \mathbf{r}) + i\kappa(\omega, \mathbf{r}), \\ \tilde{n}_\delta(\omega, \mathbf{r}) &= [n(\omega, \mathbf{r}) - 1] + i\kappa(\omega, \mathbf{r}), \\ &= n_\delta(\omega, \mathbf{r}) + i\kappa(\omega, \mathbf{r}),\end{aligned}\tag{4.84}$$

where $n_\delta(\omega, \mathbf{r})$ is the real refractive index deviation and $\kappa(\mathbf{r})$ is the extinction coefficient, which is related to the absorption coefficient α by

$$\kappa = \frac{\alpha}{2k_0}.\tag{4.85}$$

Consider a T-ray CT experiment capable of measuring the transmitted THz pulse as a function of time t , for a given projection angle and projection offset $u(\theta, l, t)$. The Fourier transform of this pulse gives $u(\theta, l, \omega)$. By removing the target and repeating the experiment $u_0(t)$ and correspondingly $u_0(\omega)$ may be measured. If the target is rotated and translated $u(\theta, l, \omega)$ may be found for sufficient projection angles to allow the filtered backprojection algorithm to be applied. Considering Eq. (4.83) it can be seen that defining

$$p_n \doteq \arg \left[\frac{u(\theta, l)}{u_0(\theta, l)} \right] / k_0 = \int_L n_\delta(\mathbf{r}) dz' = \Re \{ n_\delta(\mathbf{r}) \},\tag{4.86}$$

and,

$$p_\alpha \doteq -2 \left\| \frac{u(\theta, l)}{u_0(\theta, l)} \right\| = \int_L \alpha(\mathbf{r}) dz' = \Re \{ \alpha(\mathbf{r}) \},\tag{4.87}$$

where $\arg(x)$ denotes the phase or argument of complex valued x , $\|x\|$ denotes the magnitude or norm of the complex scalar x , and p_n and p_α are the projection data inputs to the filtered backprojection algorithm as required to reconstruct n_δ and α respectively. The reconstruction is performed at a specific THz frequency ω and the ω -dependence of $u(\theta, l)$ has been omitted in the above equations for notational simplicity.

If the target is relatively dispersionless over the terahertz frequency range, that is, its refractive index and absorption coefficient are independent of frequency, the reconstruction may be performed directly in the time domain. If $\tilde{n}_\delta$ is constant with respect to ω the inverse Fourier transform of Eq. (4.83) is given by

$$u(\mathbf{r}, t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left\{ u_0(\omega) \exp \left[ik_0 \int_L \tilde{n}_\delta dl \right] \exp[i\omega t] \right\} d\omega. \quad (4.88)$$

Substituting Eq. (4.84) and Eq. (4.85) yields

$$\begin{aligned} u(\mathbf{r}, t) &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left\{ u_0(\omega) \exp \left[\int_L ik_0 n_\delta - \frac{\alpha}{2} \right] \exp[i\omega t] dl \right\} d\omega, \\ &= \frac{1}{2\pi} \exp(-\rho) \int_{-\infty}^{+\infty} u_0(\omega) \exp(i\omega\tau) \exp[i\omega t] d\omega, \\ &= u_0(\mathbf{r}, t - \tau) \exp(-\rho), \end{aligned} \quad (4.89)$$

where τ is the pulse delay and ρ is the pulse exponential attenuation factor given by

$$\tau = \frac{1}{c} \int_{L(\theta, l)} n_\delta(x, y) dl, \quad (4.90)$$

$$\rho = \int_{L(\theta, l)} \frac{\alpha(x, y, z)}{2} dl. \quad (4.91)$$

Note that the above analysis corrects a minor error in Wang et al. (2004). In this case, the temporal profile of the THz pulse does not change, it is simply delayed by τ and attenuated by a factor $\exp(-\rho)$. The parameters τ and ρ can be easily extracted from the measured data and can be used as the input into the filtered backprojection algorithm to allow a simpler reconstruction to be performed for dispersionless targets.

4.6.4 T-ray CT Optical Design

In implementing a T-ray CT system compliant with the equations derived in Sec. 4.6.3 several factors must be considered. The system must be consistent with the stated assumptions, namely the target z extent must be smaller than the Rayleigh range of the THz beam, and the THz beam must propagate as a planar wave within the Rayleigh range. A further requirement arises from the approximation made in Eq. (4.76) that the second term may be safely neglected, that is

$$\frac{\hat{\alpha}^2 + \hat{\beta}^2}{2k_0} (d - z') < 1. \quad (4.92)$$

This requires that $\hat{\alpha}$ and $\hat{\beta}$ must be small with regard to k_0 , and the detector location d must not be far distant from the target. Consequently, $\hat{\alpha}$ and $\hat{\beta}$ are kept small by only measuring the diffracted radiation with a wave vector close to the incident wave vector. This is achieved by collecting the diffracted radiation at a point distant to the target

and only collecting the scattered radiation over a limited extent. This is illustrated in Fig. 4.36 where φ indicates the angle over which the diffracted wave vectors are captured. This angle may be related to the wave vector geometry by similar triangles,

$$\sin \varphi = \frac{\sqrt{\hat{a}^2 + \hat{\beta}^2}}{k_0}. \quad (4.93)$$

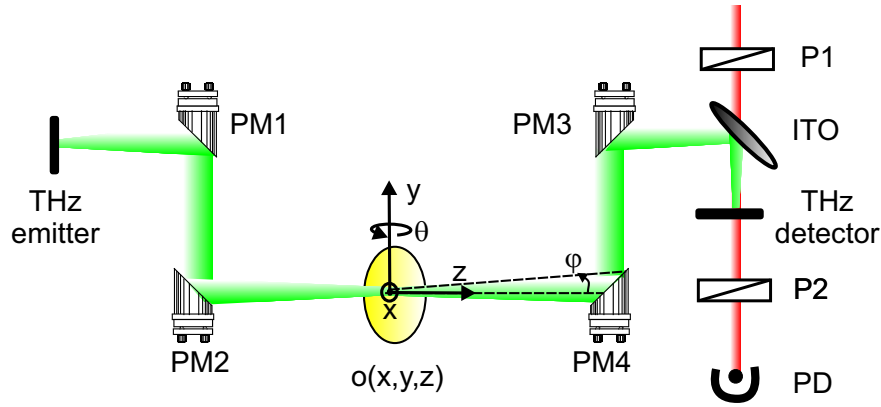


Figure 4.36. Geometry of the T-ray CT collection optics. The THz radiation is focused on the target by parabolic mirror PM2, and the scattered radiation is collected by parabolic mirror PM4. The size of PM4 relative to its focal length defines the angle φ , which determines the range of scattered wavevectors that are measured. PM3 focuses the collected THz radiation on the ZnTe detector. An ITO THz mirror allows the probe beam to copropagate with the THz beam and electro-optically detect the THz signal. After (Wang et al. 2004).

This angle is minimised by using long focal length parabolic mirrors. An aperture may be inserted close to PM4 to further reduce φ however this also reduces the measured THz signal and the SNR, as well as introducing additional distortion and diffraction of the THz beam.

Combining Eqs. (4.93) and (4.92) yields the revised requirement that

$$\frac{\sin^2(\varphi)k_0(d - z')}{2} < 1. \quad (4.94)$$

For a 250 mm focal length parabolic with a radius of 25 mm φ is approximately 5° . At a frequency of 1 THz Eq. (4.94) requires that the detector plane d be placed less than 10 mm from the target! This is extremely difficult to realise experimentally. This problem is overcome by the fact that the parabolic mirrors PM4 and PM3 act to image

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the field near the target onto the detector plane. Under the paraxial approximation these two parabolic mirrors act like a single thin lens imaging system. The effective focal length f of the equivalent thin lens system is given by

$$\frac{1}{f} = \frac{1}{f_{PM3}} + \frac{1}{f_{PM4}}, \quad (4.95)$$

where f_{PM3} and f_{PM4} are the focal lengths of the two parabolic mirrors. In this way the object plane may be chosen arbitrarily close to the target in order to satisfy Eq. (4.94).

The THz beam is focused to a diffraction limited spot size of approximately 2 mm. At a frequency of 1 THz this corresponds to a Rayleigh range of approximately 5 cm (Saleh and Teich 1991). This defines the maximum size target that can be imaged with this system given the assumptions for the reconstruction algorithm. Larger targets may be imaged by increasing the THz spot size at the focus, however this is likely to result in degradation of the spatial resolution.

4.6.5 2D T-ray CT

A 2D T-ray CT system was developed based on the standard THz-TDS scanned imaging system described in Sec. 3.3.1 and illustrated in Fig. 3.10. The target is mounted on a motion stage that allows it to be translated in x and y axes and rotated about the y axis. Long focal length (250 mm) parabolic lenses are used to provide a Rayleigh range of over 5 cm with a THz spot size of 2 mm (at 1 THz). The parabolic mirrors are positioned to allow the plane close to the target to be imaged on the ZnTe sensor as illustrated in Fig. 4.36. A THz emitter, utilising optical rectification, is used to provide a high bandwidth system using a 3 mm thick $\langle 110 \rangle$ oriented ZnTe crystal and 100 mW of pump power. The bandwidth of the system is approximately 2.2 THz. A LIA is used to detect the THz signal, the LIA time constant is set to 10 ms, and a settling time of 30 ms is used at each sample to allow the LIA to average the signal effectively. This system is limited to 2D tomographic imaging solely because of the long acquisition time. To obtain a CT image the delay stage is translated to acquire the THz temporal pulse, the x stage is then scanned, and the target rotated. For a typical experiment using relatively coarse sampling with 100 time steps, 50 x steps and 18 projection angles the acquisition time is 45 minutes. However, to perform a 3D image with this system the target must additionally be scanned in the y dimension. For 50 y steps the acquisition time increases to over 37 hours, which is obviously untenable. Section 4.6.6 discusses

an accelerated system designed for 3D CT, however this 2D CT system provides the highest possible SNR and allows the resolution and reconstruction accuracy of T-ray computed tomography to be evaluated.

Polystyrene

Polystyrene has many uses in THz systems. It has one of the lowest refractive indexes of all materials in the THz range (Zhao et al. 2002b) as well as an extinction coefficient of less than 0.5 cm^{-1} . It is relatively dispersionless over the THz band except where certain gases are used as blowing agents in its production. For instance HCFC 142b gas (1-chloro-1,1-difluoroethane) has an absorption resonance at 0.5 THz and if traces of this gas remain in the polystyrene this absorption peak is visible (Zhao et al. 2002b). Polystyrene is virtually transparent to THz radiation but absorbs in the near-infrared and higher frequencies, which allows it to be used to block the pump beam in THz experiments and be used as a substrate for imaging targets. These properties also mean that THz systems are a very attractive method for imaging polystyrene and other related foam material targets.

The physical origin of the small refractive index of foam is the low average mass density of the material, in combination with the fact that the material consists mainly of gas filled polystyrene cells with an average diameter smaller than the THz wavelengths. Bulk polystyrene has a refractive index of approximately 1.6 in the THz range (Birch 1992). As long as the wavelength of the THz radiation is much longer than the diameter of the foam cells, the refractive index is a weighted average of the refractive index of air and bulk polystyrene. As the cell size gets larger (relative to the wavelength of the radiation) it results in increased scattering of the THz radiation and increased losses (Ishimaru 1978).

The unique properties of polystyrene make it ideal for production of targets for testing T-ray CT. It has low refractive index and absorption coefficients, and is easy to machine. Extruded polystyrene was used to manufacture several targets for T-ray CT. Targets were designed to test various properties of the system. An example triangular target is shown in Fig. 4.37. For 2D T-ray CT the targets were all cylindrical providing a fixed cross-section at all heights.

T-ray computed tomography allows the complex refractive index of the target to be reconstructed. To provide a basis against which to compare the reconstructed CT results a 17 mm thick slab of polystyrene was cut and the THz response measured using a



Figure 4.37. Simple polystyrene test target. The target consists of a triangular cylinder with a side length of approximately 1 cm.

standard THz-TDS system. Figures 4.38 and 4.39 show the THz response of the polystyrene in the time and frequency domains.

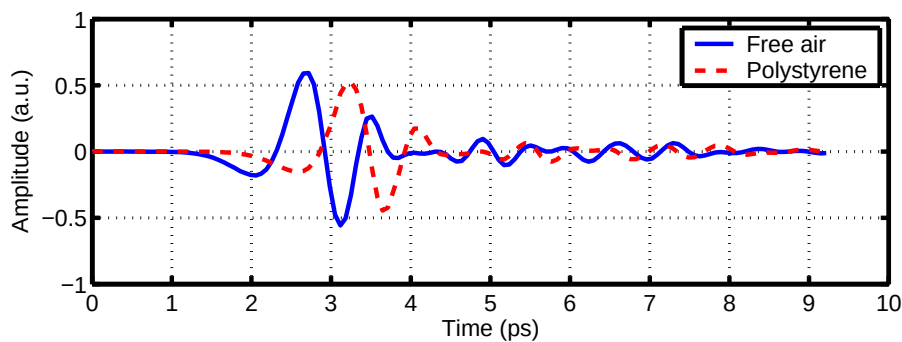


Figure 4.38. Time domain THz response of a 17 mm thick slab of polystyrene. The THz response was measured with and without the polystyrene sample in place. The polystyrene causes very little distortion of the THz waveform.

The complex refractive index of the sample was extracted using standard techniques, which are elaborated on in Appendix C and Duvillaret et al. (1996). Figures 4.40 and 4.41 show the frequency dependent refractive index and extinction coefficient of the polystyrene as calculated from the THz-TDS measurements. The results are largely dispersionless ($n = 1.011$ and $\kappa = 0.08 \text{ cm}^{-1}$).

Sinograms

The triangular polystyrene target shown in Fig. 4.37 was imaged using the 2D T-ray CT system. Very coarse imaging steps were used, particularly in the time domain, to

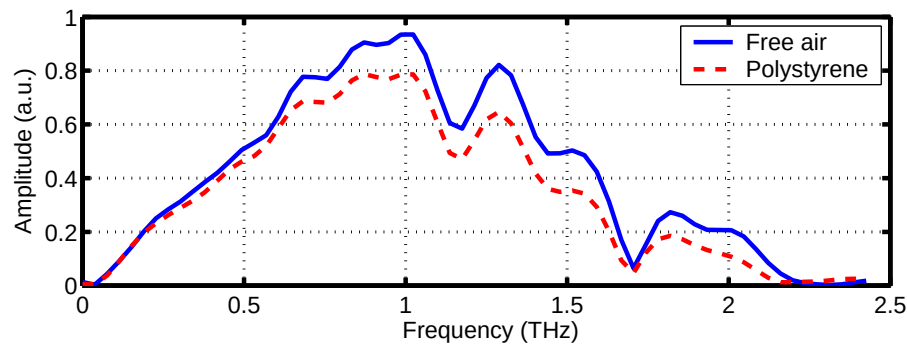


Figure 4.39. Frequency domain THz response of a 17 mm thick slab of polystyrene. A Fourier transform was performed on the signals shown in Fig. 4.38 and the spectra are shown. The polystyrene does not cause significant modification of the spectra other than a broadband absorption.

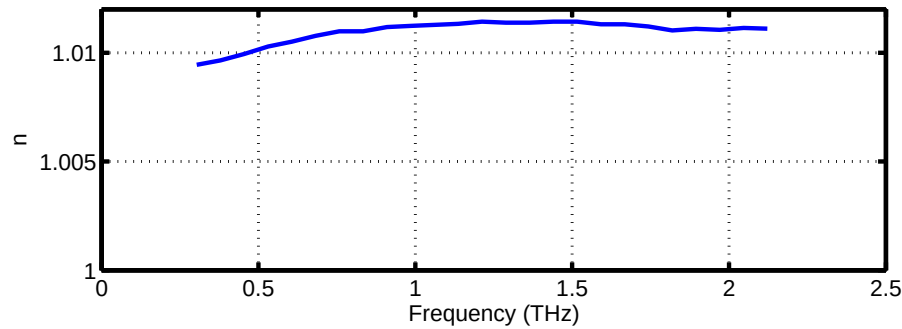


Figure 4.40. Real refractive index of polystyrene. The frequency dependent refractive index of polystyrene was extracted from the THz-TDS measurements using the method described in (Duvillaret et al. 1996). The refractive index is relatively constant across the frequency band of interest with an average value of 1.011.

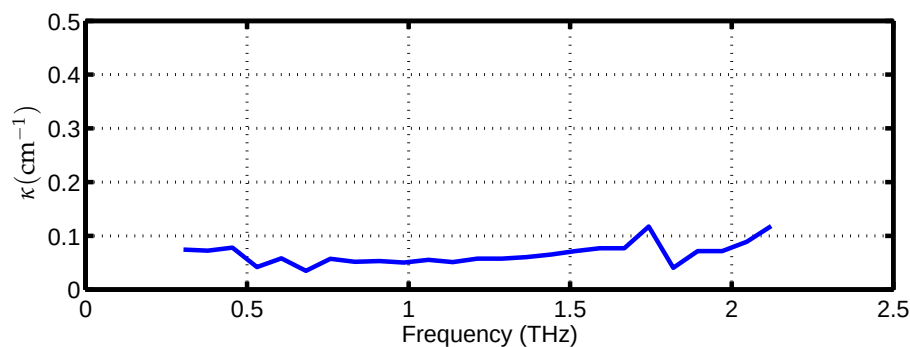


Figure 4.41. Extinction coefficient of polystyrene. The frequency dependent extinction coefficient of polystyrene was extracted from the THz-TDS measurements using the method described in (Duvillaret et al. 1996). The extinction coefficient is relatively constant across the frequency band of interest with an average value of 0.08 cm^{-1} .

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Table 4.1. CT image parameters for the triangular test target. The target is illustrated in Fig. 4.37. These parameters specify the range and resolution of the CT acquisition in each of the 3 dimensions, namely x , time, and projection angle. The time axis is implemented with a linear translation stage, and the projection angle is modified using a rotating stepper motor. Coarse step sizes were used to accelerate the image acquisition time.

Quantity	Value
X step	1 mm
X range	40 mm
time step	0.15 ps
time range	6 ps
Angular step	7.2°
Angular range	180°
LIA time constant	10 ms
Averaging time	30 ms
Total acquisition time	20 minutes

allow the target to be imaged relatively quickly. The imaging parameters are described in Table 4.1. The total acquisition time was 20 minutes.

The price of this short acquisition time is substantially increased uncertainty regarding the timing of the THz pulse. This results in noise in the reconstruction and degrades the accuracy of the reconstructed refractive index. Figure 4.42 shows the THz time domain pulses measured for three different projection angles θ .

As shown previously in this section polystyrene is relatively dispersionless over the THz range of interest. This allows the time domain reconstruction algorithms to be applied. The time domain reconstructions provide higher fidelity than the frequency domain methods because they essentially average over all frequencies. An estimate of the attenuation ρ was obtained by measuring the peak of the THz pulse $u(t)$ and the reference pulse $u_0(t)$ and inverting Eq. (4.89) such that

$$\rho = -\ln \left(\frac{u_{\text{peak}}}{u_{0 \text{ peak}}} \right), \quad (4.96)$$

where u_{peak} and $u_{0 \text{ peak}}$ are the peak amplitudes of the measured THz pulses.

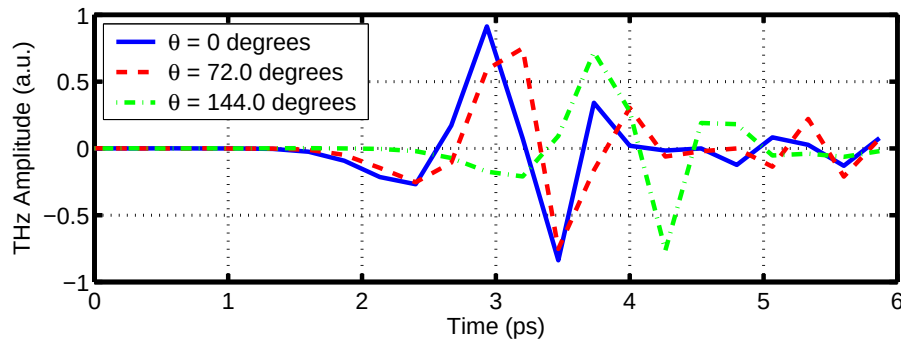


Figure 4.42. Time domain THz responses of the triangular cylinder. The THz response was measured with an extremely coarse time step to allow the measurement to be performed quickly. The THz pulse is shown for three different projection angles.

The raw data to be used in the filtered backprojection algorithm is commonly displayed in the form of a *sinogram*. A sinogram displays an image of the data as a function of projection angle θ and projection offset l . The amplitude sinogram for the triangular cylinder is shown in Fig. 4.43. This image is extremely noisy and highlights one of the problems with 2D T-ray CT. Even over this relatively short acquisition time the laser output power drifts considerably. The polystyrene target has very low absorption and therefore only results in a slight change in the amplitude of the THz pulse. This slight change is small compared to the influence of the laser fluctuation over a period of 20 minutes and this results in noisy data.

Timing Estimation

One prominent advantage of THz-TDS systems is their ability to measure the phase of the THz field as well as the amplitude. Unlike the amplitude of the ultrafast laser pulses, which exhibit strong $1/f$ noise characteristics, the phase noise, or *timing jitter* is very low (Spence et al. 1994, Sucha et al. 1999). The phase (or delay of the time domain pulse) may therefore be expected to provide a higher accuracy reconstruction than the amplitude. In THz-TDS based systems the delay of the THz pulse is commonly estimated by finding the peak of the pulse and recording the time at which the peak arrived. This method quantises the timing measurement based on the delay stage step size, Δt , which introduces a random error in the measurement. The standard deviation of this error is given by $\Delta t / \sqrt{12}$ (Proakis and Manolakis 1996). For the coarse sampling rate used for the triangle target this corresponded to an unacceptably high phase error of 43 fs.

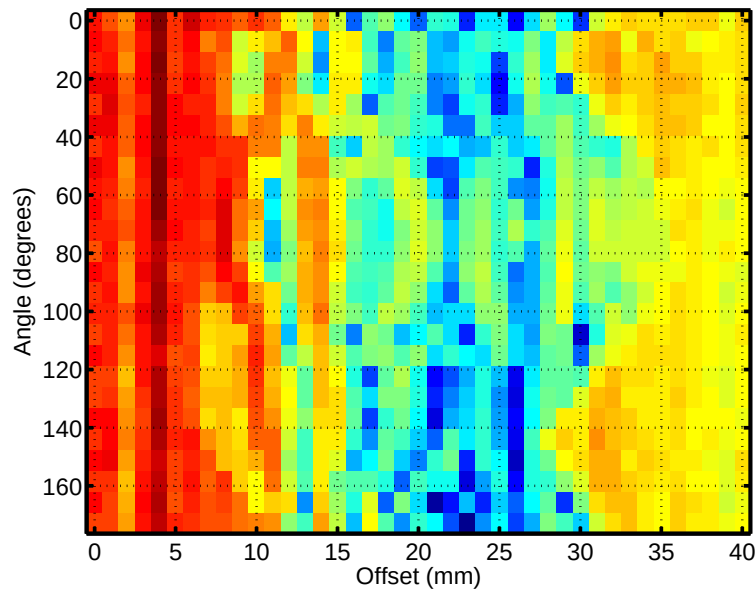


Figure 4.43. Amplitude sinogram for triangular target. The sinogram plots the amplitude of the measured THz pulse as a function of projection angle and projection offset. The amplitude sinogram exhibits considerable noise as a result of the long acquisition time, the low contrast of the target and the laser $1/f$ noise characteristics. This image uses a pseudo-colour scheme with red corresponding to the maximum received power, and violet the minimum received power. To observe the effects of noise in this image it may be contrasted with Fig. 4.45(a), which shows a timing sinogram of the same target.

An improved method of estimating the phase with an accuracy substantially higher than the sample rate was developed. This method was based on the assumption that the target is dispersionless and therefore the THz pulse shape is unchanged after propagation through the target apart from attenuation ρ and delay τ . A reference THz pulse $u_0(t)$ is measured without the target in place. To estimate the phase shift τ of a THz pulse $u(t)$ the two signals are resampled at a higher rate using lowpass interpolation. Typically the signals are resampled at 10 times the original sample rate, this results in the subsequent phase estimate being quantised with 10 times the accuracy of the previous method. The two interpolated signals are then cross-correlated, and the lag at which the cross-correlation product is maximised is taken as the estimate of the phase

delay of $u(t)$. Mathematically, this process is described by:

$$u_{\text{interp}}(m) = \sum_{t=-\infty}^{\infty} u(t) \text{sinc} \left[\frac{1}{q}(m - qt) \right], \quad (4.97)$$

$$u_{0 \text{ interp}}(m) = \sum_{t=-\infty}^{\infty} u_0(t) \text{sinc} \left[\frac{1}{q}(m - qt) \right], \quad (4.98)$$

$$u_{\text{interp}} \otimes u_{0 \text{ interp}}(m) = \sum_{k=-\infty}^{\infty} u_{\text{interp}}(k) u_{0 \text{ interp}}(k - m), \quad (4.99)$$

$$\tau_{\text{est}} = \left\langle u_{\text{interp}} \otimes u_{0 \text{ interp}}(m) \right\rangle_{\text{max lag}}, \quad (4.100)$$

where τ_{est} is the estimate for the phase delay, $u_{\text{interp}}(m)$ and $u_{0 \text{ interp}}(m)$ are equal to $u(t)$ and $u_0(t)$ after interpolation by a factor of q . The operator $\otimes$ denotes the cross-correlation as shown in Eq. (4.99) and $\langle f(t) \rangle_{\text{max lag}}$ denotes calculating the value of t at which the function f takes its maximum value.

Figure 4.44 provides an example of this algorithm. The THz projection response shown was interpolated and cross-correlated with the reference pulse. The cross-correlation result is also plotted. The lag at which the cross-correlation is maximised provides an accurate estimate of the delay between the two pulses.

A wide array of algorithms have previously been developed for estimating the timing of the peak of a pulse with subpixel accuracy. The most common methods are based on calculating the centroid, or the centre of mass of the data (Naidu and Fisher 2001, Curless 1997). Other methods are based on differentiating the time domain data and estimating the zero crossing of the derivative using interpolation (Blais and Rioux 1986). These methods were implemented and compared with the interpolated cross-correlation algorithm described above. These algorithms are based on calculating a correction to the observed peak timing. The peak of the measured pulse arrives a time t_n , but due to the quantisation process, this timing is only accurate to within half the sample period. The actual peak timing is given by $t_n + \delta_t$. These algorithms seek to estimate δ_t using the values of the THz field before and after the observed peak, $u(t_{n-1}), u(t_n), u(t_{n+1})$ etc. The algorithms are summarised below.

Gaussian Estimator. This algorithm uses the amplitude of the three highest samples around the observed peak value and assumes that the actual peak of the pulse fits a Gaussian profile. The subsample offset δ_t is estimated by (Curless 1997)

$$\delta_t = \frac{1}{2} \frac{\ln [u(t_{n-1})] - \ln [u(t_{n+1})]}{\ln [u(t_{n-1})] - 2 \ln [u(t_n)] + \ln [u(t_{n+1})]}. \quad (4.101)$$

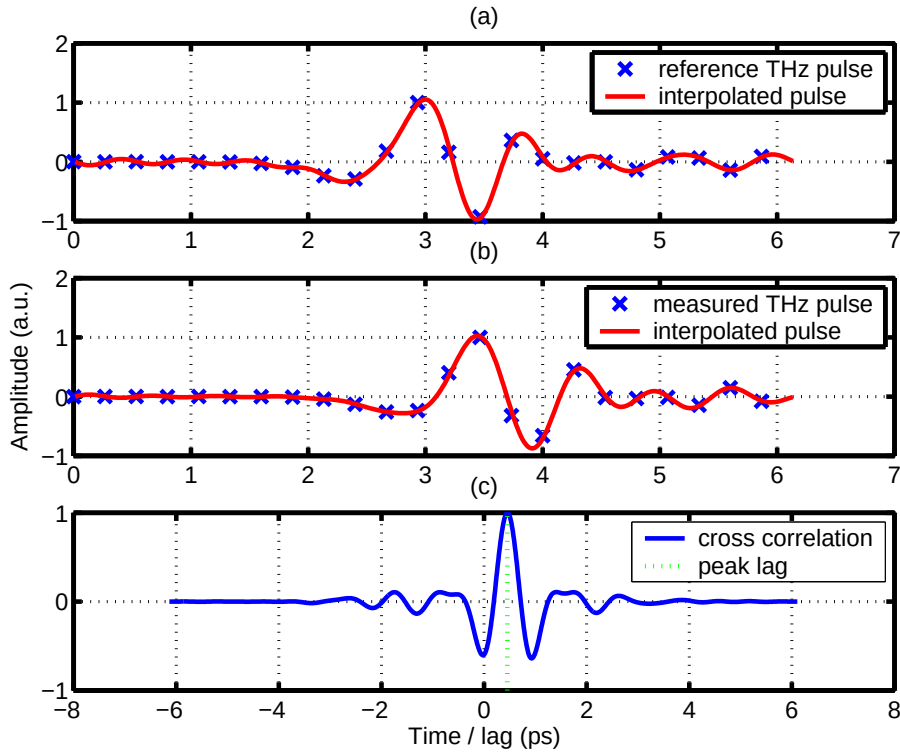


Figure 4.44. Example of τ estimation using interpolated cross-correlation. (a) This figure shows the coarsely sampled reference pulse ($\times$). The pulse is interpolated by a factor of 10 and the interpolated pulse is also shown (solid line). (b) The THz pulse after transmission through a target is shown ($\times$) along with an interpolated version of the same pulse. (c) The interpolated reference and sample pulses were cross-correlated. The lag of the peak of the cross-correlation indicates the phase delay between the two pulses.

Centre of mass. The centre of mass algorithm is again based on the assumption of a Gaussian distribution across the peak of the pulse. An estimate of the timing of the peak may then be obtained simply from the weighted average. Using 3 points around the peak results in the estimate (Naidu and Fisher 2001)

$$\delta_t = \frac{u(t_{n+1}) - u(t_{n-1})}{u(t_{n-1}) + u(t_n) + u(t_{n+1})}. \quad (4.102)$$

This algorithm can be simply extended to incorporate more points around the centre

$$\delta_t = \frac{2u(t_{n+2}) + u(t_{n+1}) - u(t_{n-1}) - 2u(t_{n-2})}{u(t_{n-2}) + u(t_{n-1}) + u(t_n) + u(t_{n+1}) + u(t_{n+2})}. \quad (4.103)$$

Linear interpolation. This algorithm assumes that the electric field varies linearly before and after the peak. Based on the three highest samples the estimate is given

by (Naidu and Fisher 2001)

$$\delta_t = \begin{cases} \frac{1}{2} \frac{u(t_{n+1}) - u(t_{n-1})}{u(t_n) - u(t_{n-1})}, & \text{if } u(t_{n+1}) > u(t_{n-1}), \\ \frac{1}{2} \frac{u(t_{n+1}) - u(t_{n-1})}{u(t_n) - u(t_{n+1})}, & \text{otherwise.} \end{cases} \quad (4.104)$$

Parabolic estimator. This estimator fits a second order function (a parabolic) to the points $u(t_{n-1})$, $u(t_n)$ and $u(t_{n+1})$ yielding the estimate (Naidu and Fisher 2001)

$$\delta_t = \frac{1}{2} \frac{u(t_{n-1}) - u(t_{n+1})}{u(t_{n+1}) - 2u(t_n) + u(t_{n+1})}. \quad (4.105)$$

Blais and Rioux method. Blais and Rioux (1986) introduced a peak estimator method based on linear filters that calculate the numerical derivative of the pulse. The algorithm estimates the zero crossing of the derivative to estimate the peak timing. They defined

$$g(t_n) = u(t_{n-2}) + u(t_{n-1}) - u(t_{n+1}) - u(t_{n+2}), \quad (4.106)$$

if $u(t_{n+1}) > u(t_{n-1})$ the estimator is given by

$$\delta_n = \frac{g(t_n)}{g(t_n) - g(t_{n+1})}, \quad (4.107)$$

otherwise it becomes

$$\delta_n = \frac{g(t_{n-1})}{g(t_{n-1}) - g(t_n)} - 1. \quad (4.108)$$

The simple triangular target was simulated using the refractive index of polystyrene determined using THz-TDS. The geometry of the T-ray CT experiment was simulated and the expected timing delay of the THz pulses was calculated for the all the projection angles and offsets used in the actual experiment. The line integral model derived in Sec. 4.6.3 was used for the forward model. This model provided the expected THz pulse delay $\tau_{\text{model}}(l, \theta)$ for each projection angle θ and projection offset l . This data was used to test the different phase estimation algorithms. The root mean square error, e_{rms} , of the different peak estimators was determined by

$$e_{\text{rms}} = \frac{1}{NM} \sum_{i=1}^N \sum_{j=1}^M \sqrt{[\tau_{\text{model}}(l_i, \theta_j) - \tau_{\text{estimate}}(l_i, \theta_j)]^2}, \quad (4.109)$$

where τ_{estimate} is the delay estimate from the chosen phase estimation algorithm, N is the number of projection offsets measured and M is the number of projection angles

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Table 4.2. RMS error in τ for a number of peak estimator algorithms. The target shown in Fig. 4.37 was modeled and the expected THz delay for each projection path was calculated. The measured data was processed to calculate the THz delay using each of the techniques listed in the table. The estimated experimental delay was compared with the expected delay to calculate the accuracy of the estimation algorithm according to Eq. (4.109).

Algorithm	e_{rms} (fs)
Timing of peak	49
Linear estimation	32
Parabolic estimation	25
Centre of mass	22
Blais Rioux	18
Interpolated cross-correlation	11

measured. The mean square error for each of the peak estimator algorithms are shown in Table 4.2.

The interpolated cross-correlation algorithm developed in this Thesis proved substantially more accurate than any of the other methods tested. This improvement is attributed to the fact that the cross-correlation method incorporates additional information on the shape of the THz pulse based on the reference pulse $u_0(t)$. All of the other methods assume that the peak of the pulse follows a particular distribution, the centroid and Blais Rioux algorithms assume a Gaussian distribution and perform marginally better than the parabolic estimator, which assumes that the peak of the THz pulse can be approximated by a parabola – but none of these other methods make use of $u_0(t)$. Additionally, the cross-correlation algorithm incorporates all the measured data from the whole THz pulse, while the other algorithms are based solely on the samples near the main peak of the pulse. This additional data provides increased robustness to noise.

Figure 4.45 compares the timing sinograms produced using the interpolated cross-correlation algorithm and the standard method of using the time of arrival of the peak of the pulse. The interpolated cross-correlation method results in a significantly improved sinogram. This in turn results in improved reconstructed images.

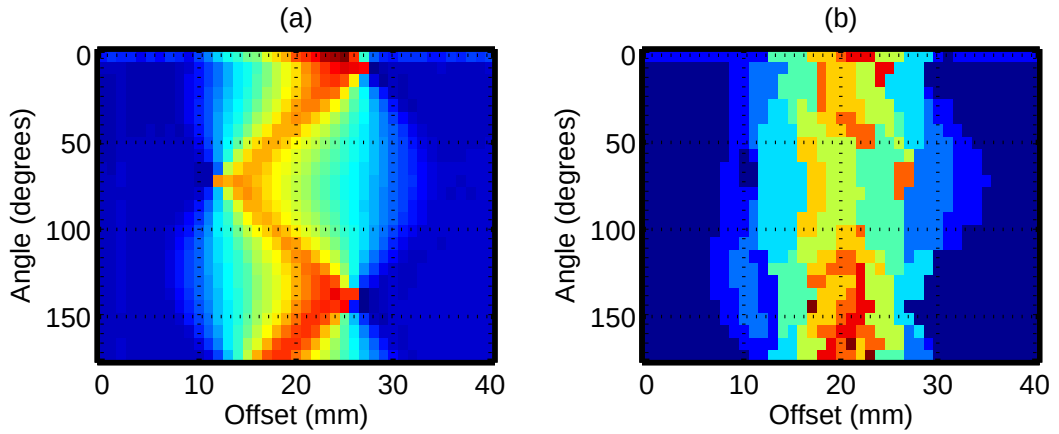


Figure 4.45. Timing sinograms for the triangular target. (a) The timing of the measured THz pulses was estimated using the interpolated cross-correlation algorithm. The timing is plotted against the projection angle and offset. (b) The timing was estimated by time of arrival of the peak of the pulse. The coarse sampling rate resulted in severe quantisation errors, which introduce artifacts and noise into the reconstructed image. In both figures red corresponds to maximum delay, followed by orange, yellow, green, blue, indigo and violet in order of decreasing delay.

Time Domain Target Reconstruction

The low extinction coefficient of the polystyrene target and the high $1/f$ amplitude drift of the laser prevented a successful reconstruction of the extinction coefficient of the target. However, the interpolated cross-correlation algorithm allowed the timing of the THz pulses to be estimated with high accuracy and the timing data could then be used to reconstruct the real refractive index of the target.

The delay τ was estimated from the projection data and the filtered backprojection algorithm (Sec. 4.6.2) was applied to reconstruct the target. The reconstructed cross-section of the triangular target is shown in Figs. 4.46 and 4.47. The reconstructed refractive index $n(\mathbf{r})$ fluctuates over the surface of the reconstructed triangle but $n_\delta = n - 1$ is within 25% of the expected value of 0.011.

To further test the capabilities of the T-ray CT system a more complicated target was fabricated and imaged. The letters 'T', 'H' and 'Z' were drilled into a rectangular cylinder of polystyrene as shown in Fig. 4.48.

The target was imaged using resolutions of 0.6 mm, 7.2° and 0.1 ps in the l, θ and time axes respectively. This resulted in a total acquisition time of 1.25 hours. Table 4.3 provides a summary of the test conditions.

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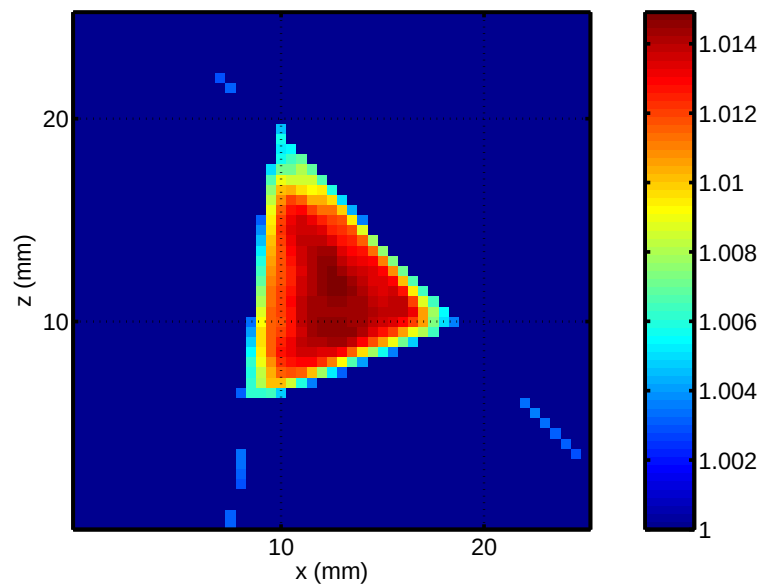


Figure 4.46. Reconstructed cross-section of the triangular polystyrene target . The timing of the THz pulses was estimated using the interpolated cross-correlation algorithm and the filtered backprojection algorithm was then used to reconstruct the real refractive index of the target. The actual refractive index of the polystyrene target is 1.011. The reconstructed image is quite accurate in both the structural and dielectric properties of the target. The colorbar on the right shows the refractive index corresponding to each colour in the image.

Table 4.3. T-ray CT imaging parameters for the ‘THZ’ polystyrene target. The target is illustrated in Fig. 4.48. These parameters specify the range and resolution of the CT acquisition in each of the 3 dimensions, namely x , time, and projection angle. The time axis is implemented with a linear translation stage, and the projection angle is modified using a rotating stepper motor.

Quantity	Value
X step	0.6 mm
X range	60 mm
Time step	0.1 ps
Time range	6 ps
Motor step	7.2°
Motor range	180°
LIA time const	10 ms
Averaging time	30 ms
Acquisition time	75 minutes

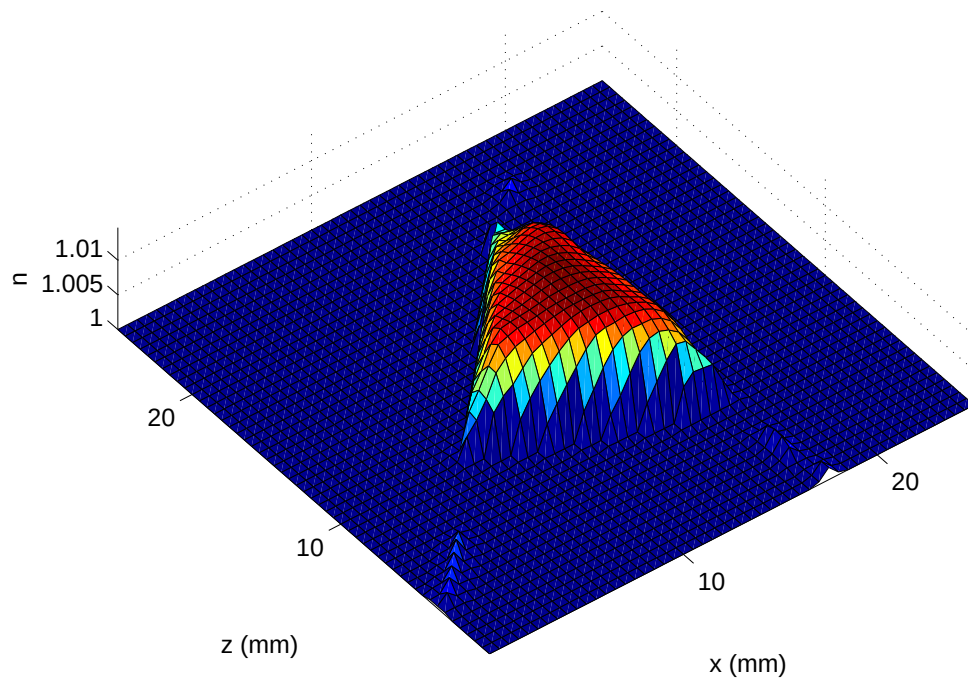


Figure 4.47. 3D visualisation of the reconstructed cross-section of the triangular polystyrene target. The vertical dimension in the image depicts the reconstructed refractive index of the material.



Figure 4.48. Polystyrene block with the letters 'THZ' drilled into it. This figure shows an optical image of the polystyrene block target. The target has dimensions of $45 \times 25 \times 35$ mm (length $\times$ width $\times$ height) and the letters each have a thickness of approximately 2 mm.

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This target has a more complicated structure than the first example considered and resulted in additional scattering of the THz radiation and a less accurate reconstruction. The timing sinogram and timing reconstruction are shown in Figs. 4.49 and 4.50 respectively. The reconstructed shape of the target is reasonably accurate, however several artifacts are visible in the reconstruction.

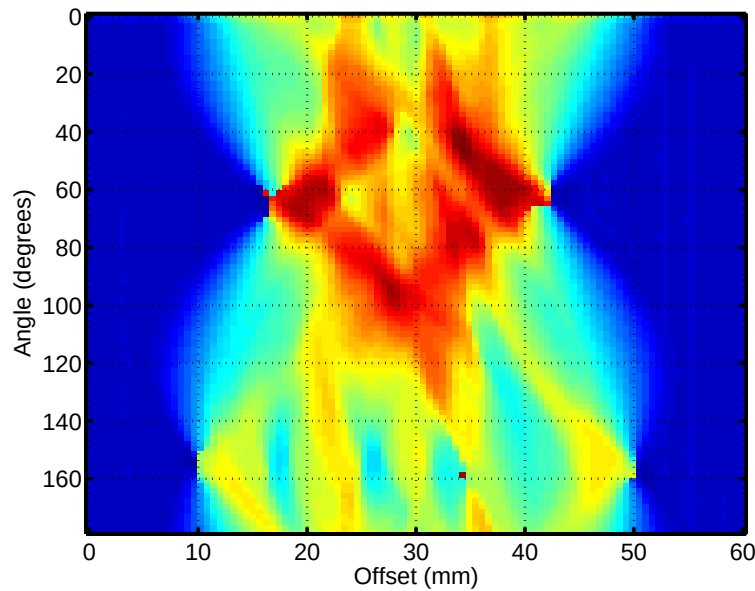


Figure 4.49. Timing sinogram for the 'THZ' target. The timing of the measured THz pulses was estimated using the interpolated cross-correlation algorithm. The timing is plotted against the projection angle and offset. The target is shown in Fig. 4.48. The relative delay of the pulse is indicated by the colour of each pixel. Red corresponds to maximum delay, followed by orange, yellow, green, blue, indigo and violet in order of decreasing delay.

Resolution

An important parameter of any imaging system is the achievable resolution. The resolution of standard X-ray CT systems is given by $\sqrt{\lambda L}$, where λ is the wavelength of the incident radiation and L is the sample to detector distance (Gbur and Wolf 2001). For example, a typical X-ray CT system operating at a wavelength of $1 \text{ \AA}$, and a target to detector distance of 0.5 m has a resolution limit of $7 \text{ }\mu\text{m}$. A number of additional issues such as detector spacing and X-ray scattering commonly reduce the resolution even further. An important distinction between the T-ray CT system described here, and standard CT systems is that the T-ray CT system is coherent. By measuring the phase

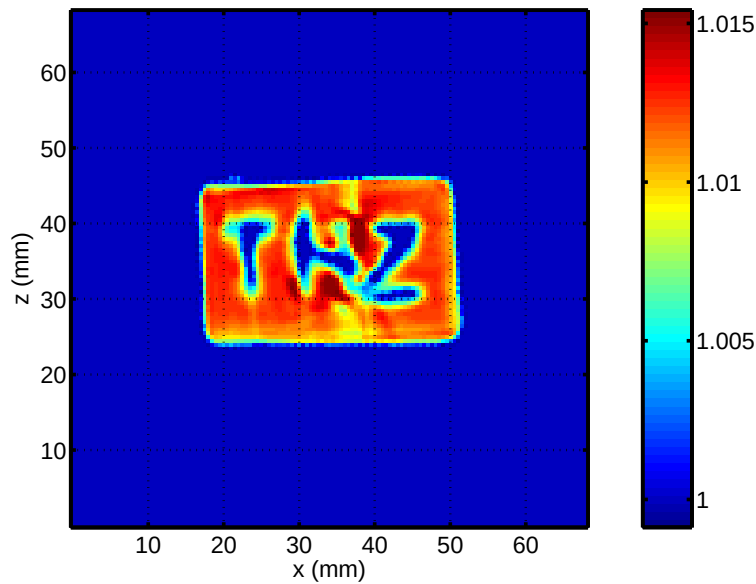


Figure 4.50. Reconstructed cross-section of the 'THZ' polystyrene target. The reconstructed image is again, quite accurate in both the structural and dielectric properties of the target. Some artifacts are visible on the right of the letter 'H' resulting from the additional complexity of this target. The colour-bar on the right maps the colours in the image to the reconstructed refractive index.

of the THz field, and using parabolic mirrors to image the field close to the target, the usual resolution limit of $\sqrt{\lambda L}$ does not apply (Wang et al. 2004).

A further polystyrene target was constructed to investigate the resolution of T-ray CT. The target is shown in Fig. 4.51. Several holes were drilled into a polystyrene cylinder. The hole spacing was varied and the hole diameter was approximately 2 mm.

The resolution test target was imaged with the image parameters shown in Table 4.4. A relatively fine step size was used in each dimension. This resulted in a long acquisition time of over 2.5 hours, but allowed the resolution limit of the system to be investigated.

The timing was used to reconstruct the target and the reconstruction is shown in Figs. 4.52 and 4.53. The reconstruction accuracy is excellent. All holes are resolved including the two closest in the upper right of Fig. 4.52. These holes are separated by less than 0.5 mm and indicate that the resolution of the system exceeds 0.5 mm. For the T-ray CT system $\lambda = 0.3$ mm, and $L = 400$ mm, therefore the traditional (incoherent) resolution limit is $\sqrt{\lambda L} \approx 11$ mm. The resolution of the developed coherent T-ray CT system is approximately 0.5 mm, which exceeds the traditional limit by over an order of magnitude.

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Figure 4.51. Detailed polystyrene resolution test target. An optical image of a target with 2 mm diameter holes drilled into a polystyrene cylinder with varying interhole distances.

Table 4.4. T-ray CT imaging parameters for the resolution test target. The target is shown in Fig. 4.51.

Quantity	Value
X step	0.5 mm
X range	60 mm
Time step	0.66 ps
Time range	6.6 ps
Motor step	7.2°
Motor range	180°
LIA time const	10 ms
Averaging time	30 ms
Acquisition time	150 minutes

An important distinction should be drawn between the ability to resolve two targets in the reconstructed image and the ability to accurately reconstruct their refractive index. Figure 4.55 shows the reconstructed refractive index along the line A'-A in Fig. 4.54. While all 5 holes can be identified along the line, the refractive index within the hole should be 1, while the refractive index of the polystyrene should be 1.011. The T-ray CT reconstruction algorithm is based on the Rytov approximation, which assumes that the phase of the diffracted field (and therefore the refractive index of the target) varies slowly relative to the wavelength. As a result, sharp discontinuities in the refractive index of the target are not reconstructed accurately. This causes the reconstructed image

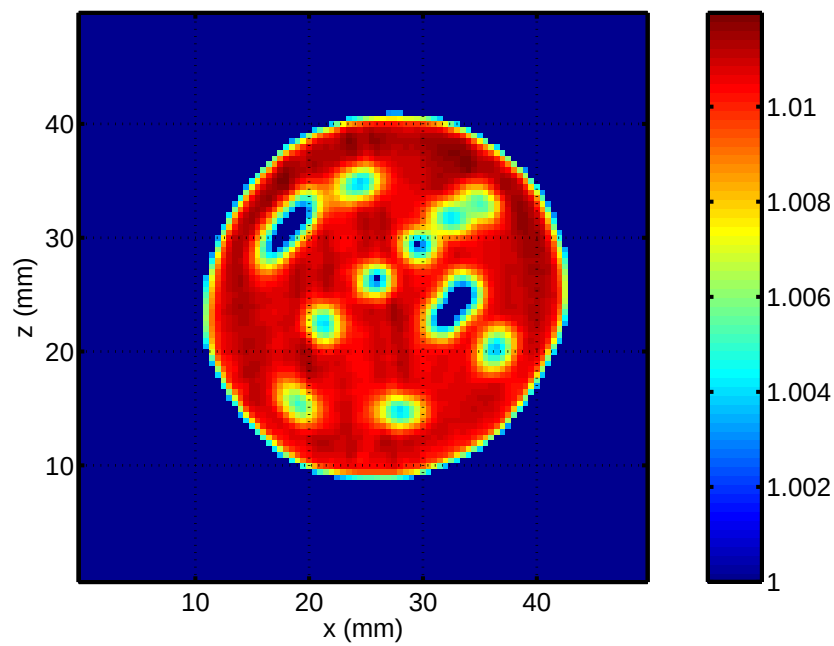


Figure 4.52. Reconstructed cross-section of the resolution test target. The two holes in the upper right corner of the image are separated by 0.5 mm of polystyrene. This indicates that the resolution limit of the system is better than 0.5 mm.

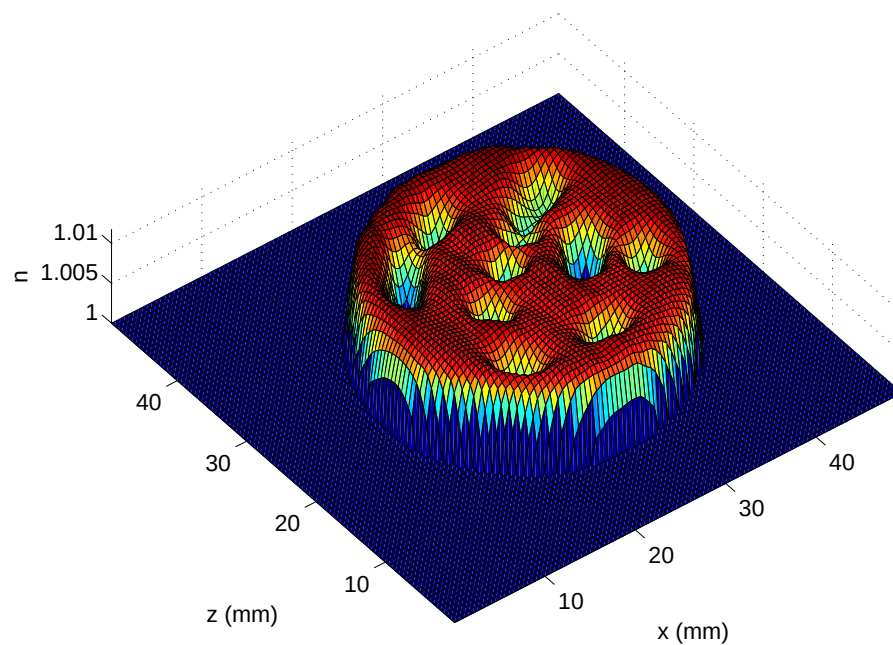


Figure 4.53. 3D visualisation of the reconstructed cross-section of the resolution test structure. The vertical dimension in the image depicts the refractive index of the material. The original target is shown in Fig. 4.51.

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to be low pass filtered and inaccuracies in the reconstructed index on the boundaries of objects.

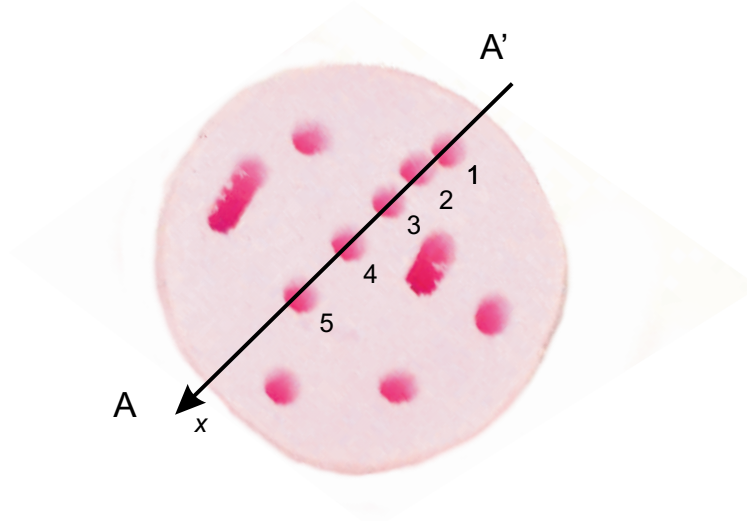


Figure 4.54. Top view of polystyrene resolution test target. The line A'-A is drawn through 5 holes with varied interhole spacing.

Frequency Domain Target Reconstruction

As derived in Sec. 4.6.3 the reconstruction can also be performed in the frequency domain. In this case the input to the filtered backprojection is either the deconvolved amplitude of the THz pulse or the deconvolved phase at a given frequency. The process of deconvolution is commonly employed in THz-TDS systems (Mittleman et al. 1996, Ferguson et al. 2002e). It is used as the first step in extracting the refractive index from the measured THz pulses (Duvillaret et al. 1996). Conceptually, the THz pulse measured in a THz-TDS experiment is dependent on the properties of the THz source and detector, as well as the properties of the target. Deconvolution uses a reference pulse, measured without the sample in place, to isolate the influence of the target on the THz pulse from these other effects. Deconvolution is discussed in more detail in Ch. 5.

One critical factor in the deconvolution process is that of estimating the phase of the Fourier coefficients. The Fourier transform of the THz pulses yields the complex Fourier coefficients $(a + ib)$ at each frequency. The phase ϕ of these Fourier coefficients is given by

$$\phi = \arctan\left(\frac{b}{a}\right), \quad (4.110)$$

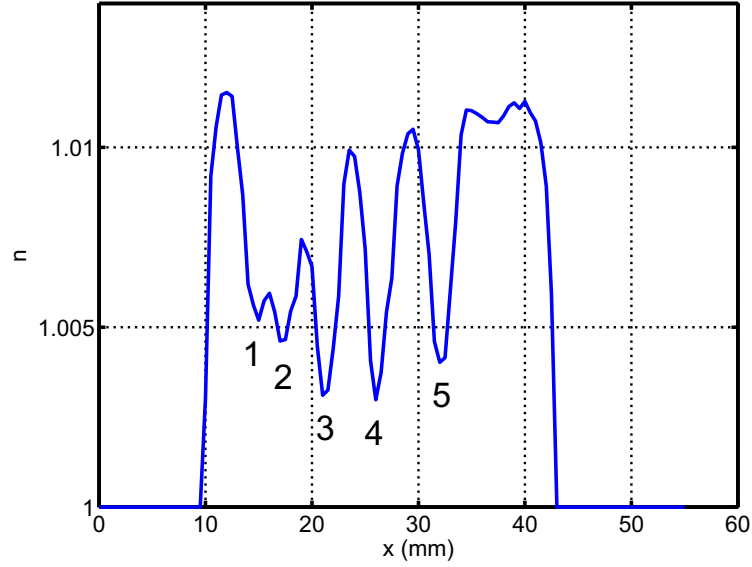


Figure 4.55. Reconstructed refractive index along line A'-A in Fig. 4.54. All 5 holes are identifiable in the reconstructed profile, including the two on the left, which are separated by less than 0.5 mm. However, the refractive index profile is low pass filtered in the reconstruction process and the refractive index is not accurately recovered.

however this yields a value between $-\pi$ and π , while the actual phase is not restricted to this range. The actual phase is given by $\phi + 2n\pi$, where n is an unknown integer. The process of unwrapping attempts to determine n by considering ϕ as a function of frequency. Commencing with the first frequency component, where n is assumed to be zero, and iteratively considering higher frequency components, wherever the phase jumps by more than π , n is incremented (or decremented) such that the difference between two adjacent phases is less than π . This method works well provided that the data is relatively noise-free. However, when noise causes fluctuations in ϕ this may cause the phase to be unwrapped incorrectly. This is a particular problem for THz-TDS systems because most THz sources are band-limited and often have low power at frequencies below 0.2 THz. This causes the phase at these frequencies to be unwrapped incorrectly, and because the unwrapping procedure is iterative, this results in the errors being propagated to all higher frequencies.

This problem is addressed in this Thesis by starting the unwrapping procedure at a frequency of 0.2 THz where the SNR is typically high enough to allow an accurate phase measurement. The phase is unwrapped over the range of 0.2 THz to 0.4 THz. The slope of the phase in this range is then extrapolated over the range 0.2 THz to 0.

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Thus the phase is assumed to be linear over low frequencies where the noise is typically too high to allow the phase to be accurately determined. This allows an estimate of the phase at 0.2 THz to be obtained and the standard phase unwrapping procedure may then be employed.

Figure 4.56 shows a comparison of the two unwrapping procedures. A THz pulse through the centre of the target shown in Fig. 4.51 was used. The polystyrene target is known to be relatively dispersionless so the linear approximation is known to be accurate. The standard unwrapping algorithm resulted in an error of over 5.5 radians over all frequencies!

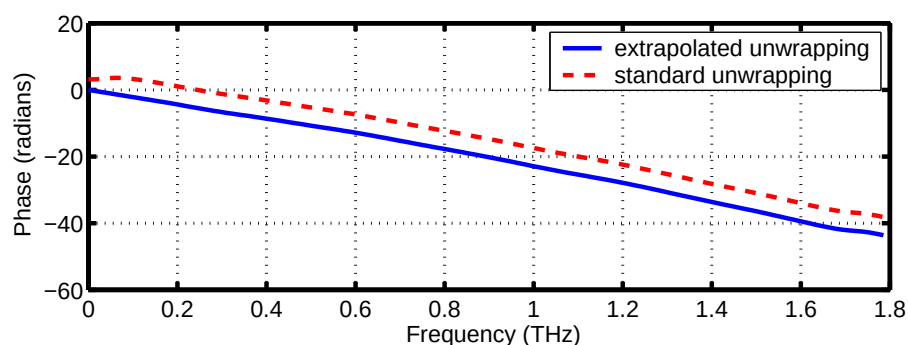


Figure 4.56. Deconvolved phase as a function of frequency. The frequency dependent phase of a typical THz projection pulse is plotted. Normal phase unwrapping is contrasted with extrapolated phase unwrapping. The extrapolated phase was calculated by unwrapping the phase from 0.2-0.4 THz and extrapolating the phase from this region from 0.2 THz to 0. The extrapolated unwrapping method results in a significant improvement.

For the polystyrene targets, the Fourier amplitude reconstruction suffered the same problems as the time domain amplitude reconstruction. The laser noise obscured the target response to a point where an accurate reconstruction was not possible. However the Fourier phase reconstruction proved very accurate and could be performed over all frequencies from 0.2 THz up to 2.0 THz. Figure 4.58 shows the phase reconstruction for a number of different frequencies based on the sinograms shown in Fig. 4.57.

The frequency dependent refractive index of the target can be determined using T-ray CT provided the refractive index is measured away from a material boundary. A pixel was chosen on the centre right of the resolution test target away from any holes. The target was reconstructed at all available frequencies from 0 to 3 THz and the refractive index at the selected pixel is shown in Fig. 4.59. The refractive index of polystyrene was determined using standard THz-TDS (see Fig. 4.40) and this is also plotted for

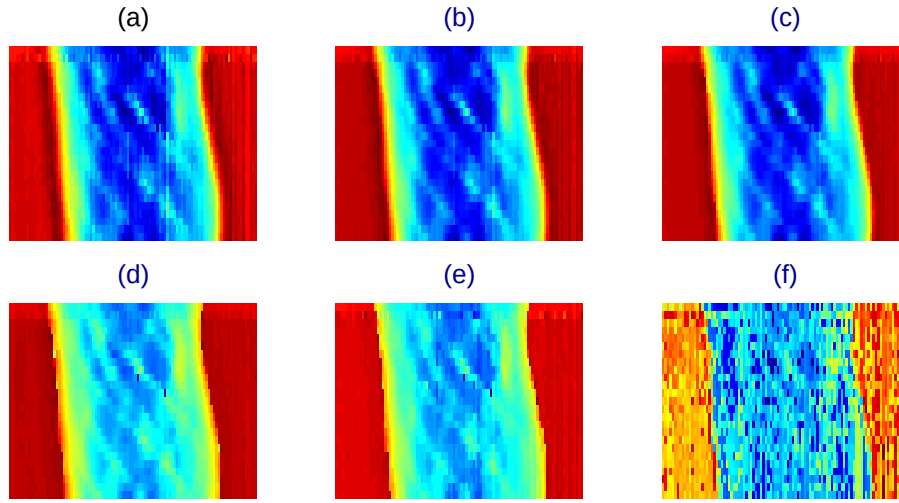


Figure 4.57. Fourier phase sinograms for the resolution target. The phase of the deconvolved THz response at frequencies of (a) 0.2 THz, (b) 0.6 THz, (c) 1.0 THz, (d) 1.4 THz, (e) 1.8 THz, and (f) 2.2 THz, were used to generate sinograms. The horizontal axis is the projection offset (0 to 50 mm) and the vertical axis is the projection angle (0 to 180°). The colour of each pixel indicates the Fourier phase. Red corresponds to the maximum phase followed by orange, yellow, green, blue, indigo and violet in order of decreasing phase.

reference. The T-ray CT result shows very good agreement with the expected refractive index over the frequency range 0.5 to 2.0 THz.

Image Quality

The image quality of the reconstructed images can be quantitatively compared by comparing them with the optical image of the target. The optical image shown in Fig. 4.54 was imported and thresholded to remove the influence of shadow. The polystyrene areas were assumed to have an index of 1.011 while the holes and surrounding area were assumed to have an index of 1.0. The image was discretised on the same size grid employed for the CT reconstructions. This actual image of the target is denoted $o(x, z)$ while the reconstructed image is denoted $\hat{o}(x, z)$. The RMS error in the reconstructed image is given by

$$e_{\text{rms}} = \frac{1}{N^2} \sum_{i=1}^N \sum_{j=1}^N \sqrt{(o(x_i, z_j) - \hat{o}(x_i, z_j))^2}, \quad (4.111)$$

where N^2 is the number of pixels in the square reconstruction grid. The reconstructed images at each frequency can now be compared quantitatively by calculating the RMS

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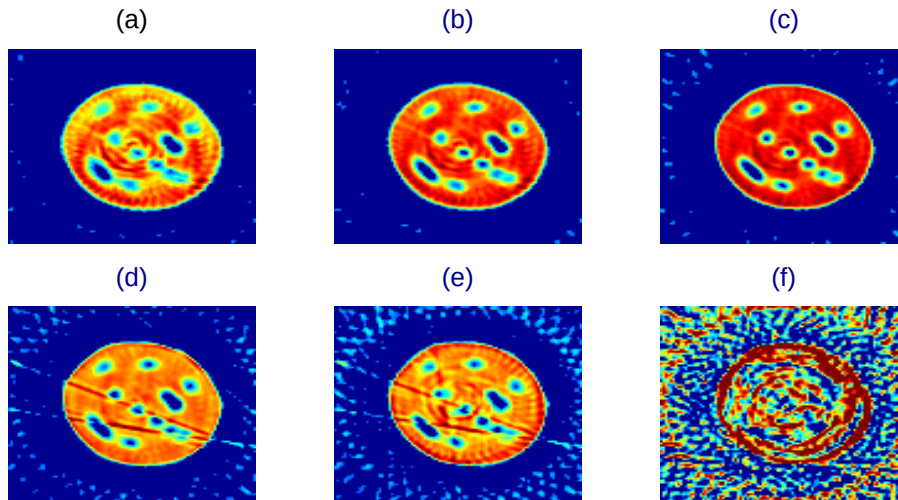


Figure 4.58. Reconstructed cross-sections using the Fourier phase. The sinogram data in Fig. 4.57 was used to reconstruct the target shown in Fig. 4.51 at different frequencies (a) 0.2 THz, (b) 0.6 THz, (c) 1.0 THz, (d) 1.4 THz, (e) 1.8 THz, and (f) 2.2 THz. The reconstructions are plotted in the $x - z$ plane from 0 to 50 mm. Subfigures (d) and (e) exhibit a common artifact found in CT images. Phase unwrapping errors resulted in several pixels having a much larger unwrapped phase than surrounding pixels, as seen in Fig. 4.57 (d) and (e). The filtered backprojection algorithm propagates these errors along the projection line resulting in the dark line artifacts.

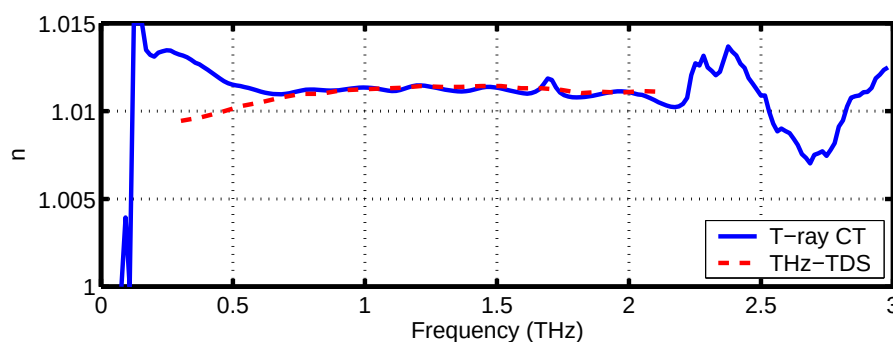


Figure 4.59. Reconstructed frequency dependent refractive index. The target shown in Fig. 4.51 was reconstructed using the Fourier phase at frequencies from 0 to 3 THz. A single pixel was selected from the centre right of the target and its reconstructed refractive index is plotted against frequency. The refractive index of polystyrene as determined using standard THz-TDS is also shown.

error of each. These are plotted in Fig. 4.60. The reconstructed image quality is closely related to the SNR of the THz measurements and it is high over the bandwidth of the THz pulses but falls off at both high and low frequency limits.

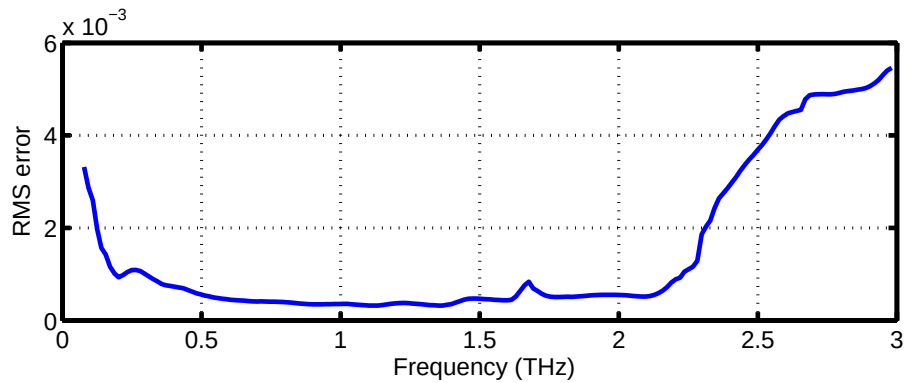


Figure 4.60. Variation in reconstructed image quality with frequency. The resolution test target of Fig. 4.51 was reconstructed using the phase at all available frequencies. Each reconstructed image was compared with the reference image of the target and the RMS error in the image was calculated. The error is very low over the useful bandwidth of the THz system (0.3 to 2.2 THz) but increases outside of this range as the SNR of the measured data increases.

4.6.6 3D T-ray Computed Tomography

The T-ray CT system described in the previous section is capable of obtaining high resolution, high fidelity cross sectional images of a target, however because of its acquisition speed is largely limited to obtaining 2D images. To demonstrate 3D imaging the same tomographic design principles were applied to the chirped probe pulse THz imaging system described in Sec. 3.3.3. This system is capable of obtaining the full THz time domain response in 60 ms, and is almost two orders of magnitude faster than the scanned THz imaging system used for 2D T-ray CT. The chirped probe pulse THz imaging technique does not require MHz laser repetition rates and thereby facilitates the use of high power regeneratively amplified lasers.

The imaging system shown in Fig. 3.21 was used for 3D T-ray CT. The target is mounted on a rotation stage, a 250 mm focal length parabolic mirror is used to focus the THz radiation to a spot size of 2 mm at the target and the parabolic mirrors after the sample are positioned to image the field from a plane near the target onto the ZnTe sensor. To

4.6 T-ray Computed Tomography

ensure a high SNR a PCA THz source is used. The electrodes are separated by 16 mm and a bias of 2 kV is applied.

The optical probe pulse is linearly chirped and temporally stretched to a pulse width of 30 ps, using a grating pair with a separation of 4 mm, an incident angle of 51° and a grating constant of $10\text{ }\mu\text{m}$. The THz pulse modulates the probe pulse via the EO effect and is recovered with a spectrometer (SPEX 500M) and CCD camera (PI-Pentamax). The CCD exposure time is set to 15 ms. This allows a THz pulse to be measured in approximately 60 ms and provides a signal-to-noise ratio of approximately 100. The bandwidth of the system is limited by the chirped pulse detection technique to approximately 1 THz. The CCD resolution results in a sampling period of 0.15 ps and a spectral resolution of 17 GHz.

Coordinate System

The 3D T-ray CT system allows a four-dimensional data set to be acquired in terms of $\{\theta, l, y, t\}$ where θ is the projection angle, l is the horizontal offset from the axis of rotation, z is the vertical dimension parallel to the axis of rotation and t is the time. We desire a reconstruction of the object's optical properties in terms of $\{x, y, z, \omega\}$ where x, y and z are the coordinate axes of the object and ω is the frequency. The coordinate system is illustrated in Figure 4.61.

3D Reconstruction

The chirped probe beam has a maximum pulse length of approximately 30 ps, this requires the use of very thin targets so that the THz pulse remains within the detection window. The chirped probe detection technique also severely limits the high frequency response as discussed in Sec. 3.3.3.

Despite these limitations this system allows 3D targets to be imaged within reasonable acquisition times. The target shown in Fig. 4.62 consists of a sheet of polyethylene bent into an 'S' shape. A coarse sampling step of 1 mm in the z and l dimensions was used to obtain projection images for each 10° angular increment. The target was imaged at 20 different heights and the total acquisition time was less than 13 minutes.

The time domain phase delay τ was estimated using the interpolated cross-correlation algorithm described previously and this data was used to reconstruct the cross-section of the target as shown in Fig. 4.63. The SNR of this 3D system is one order less than

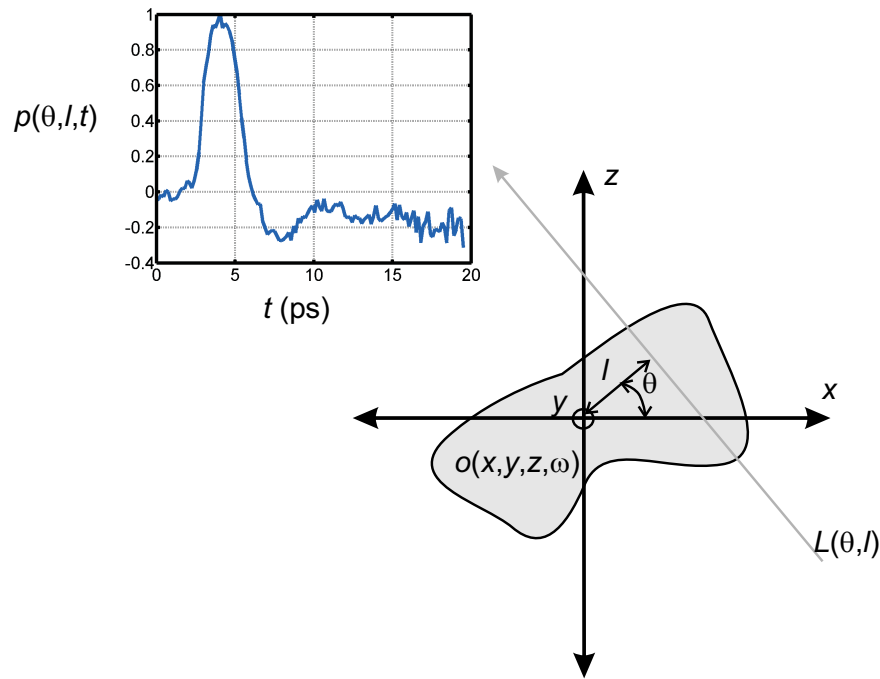


Figure 4.61. The coordinate system used for T-ray CT. The dimensions x, y and z form the standard Cartesian coordinates (y is out of the page). The object is rotated about the y axis. The THz beam propagates through the target at an angle θ to the x axis and offset l from the axis of rotation. The inset shows the projection data, a typical THz pulse as a function of time, $p(\theta, l, t)$, after propagation through a target. The line $L(\theta, l)$ defines a straight line through the target, which has a frequency dependent object function $o(x, y, z, \omega)$.

that of the 2D CT system and the reconstruction quality is therefore reduced. However, the target is still reconstructed accurately and the resolution is sufficient to reconstruct the scotch tape used to hold the polyethylene in place.

A 3D image can be formed by reconstructing each horizontal slice and surface rendering them as illustrated in Fig. 4.64. The 3D image is formed by rendering the isosurface formed at 50% of the peak reconstructed refractive index.

T-ray computed tomography is restricted in biomedical applications by the severe absorption of THz by moist tissue. However some biological tissues, such as bone, have more moderate absorption coefficients, which makes transmission mode imaging feasible. A section of a turkey femur was prepared by soaking it in acetone for 6 hours to ensure maximal transmission of THz radiation. The sample was imaged using a sampling step of 1 mm in the x and y dimensions to obtain projection images for each 10° angular increment. A frequency independent reconstruction was performed using



Figure 4.62. Top view of a 0.6 mm thick polyethylene sheet folded into an 'S' shape. The polyethylene was held in place using scotch tape. The sample was mounted such that the THz beam propagated in the plane of the paper and the sample was rotated about the y-axis (the axis pointing out of the page).

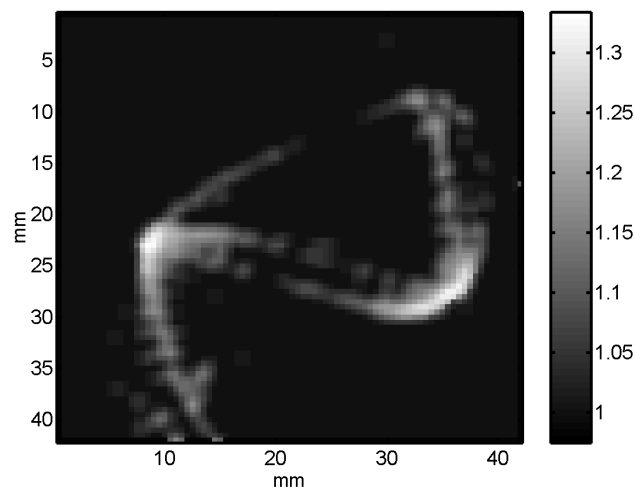


Figure 4.63. A time domain reconstruction of the sheet of polyethylene. The measured data was reconstructed using the filtered backprojection algorithm. The timing τ of the THz pulses was used as the input to the algorithm. The greyscale-bar on the right, maps the reconstructed refractive index to the greyscale shades in the image. The original target is shown in Fig. 4.62.

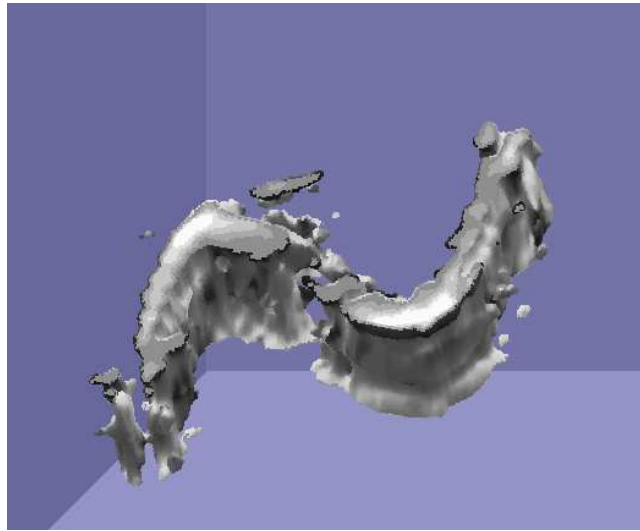


Figure 4.64. A 3D reconstruction of the sheet of polyethylene. The measured data was reconstructed using the filtered backprojection algorithm. A 2D reconstruction was performed on each horizontal slice of the data. The reconstructions are combined and surface rendered. The solid object corresponds to the regions where the reconstructed refractive index is greater than 1.15. The solid object is 3D rendered with shadowing provided by a simulated light source in the front left of the image.

the peak amplitude of the THz pulses to calculate ρ , and ρ was used as the input to the filtered backprojection algorithm. Figure 4.66 shows an optical image of the bone sample. The polystyrene targets considered in Sec. 4.6.5 had a very small absorption coefficient and the amplitude reconstruction was not successful as the laser noise dominated the amplitude measurements. However, the bone sample considered here has a significantly higher absorption coefficient – in excess of 8 cm^{-1} . Together with the significantly enhanced acquisition speed of this 3D T-ray CT system, this enabled an amplitude based reconstruction to be performed. The amplitude sinogram for a single cross-section is shown in Fig. 4.65.

A 2D reconstruction was performed for each horizontal slice of the bone and these slices were combined to form a 3D rendered image as illustrated in Fig. 4.67. The rendered isosurface threshold was constructed by joining the pixels where the reconstructed absorption coefficient fell to 50% of the peak absorption coefficient. This resulted in a reconstructed bone diameter of 22 mm compared to the measured diameter of 18 mm, measured across the widest part of the bone. The irregular surface of the reconstructed image is a result of the surface rendering technique. Variations in the reconstructed absorption as a result of noise or actual variations in the bone's absorption

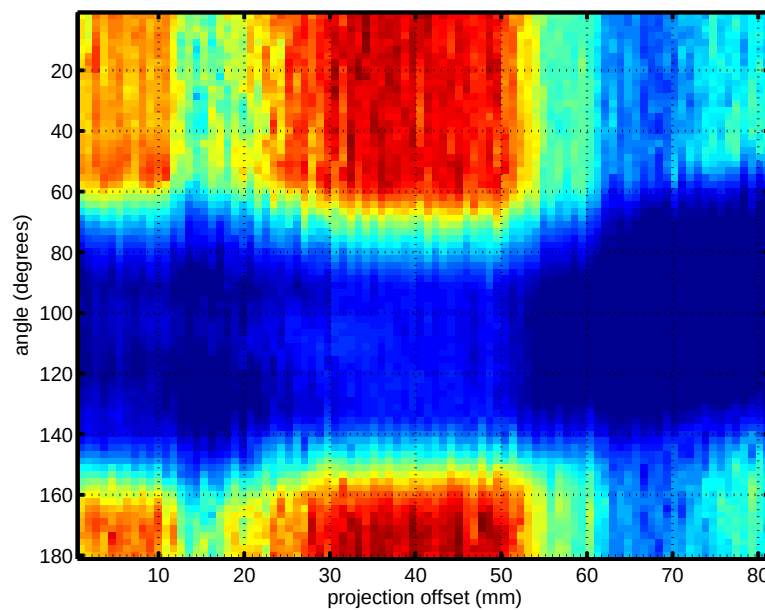


Figure 4.65. Amplitude (ρ) sinogram for the turkey femur. The absorption coefficient ρ was calculated as a function of θ and l for a single horizontal slice. The absorption of the bone is sufficient to allow a reasonable reconstruction despite the $1/f$ laser noise. The colour of each pixel corresponds to the absorption for that projection. Red corresponds to minimum absorption, followed by orange, yellow, green, blue, indigo and violet in order of increasing absorption.

coefficient result in an irregular isosurface. The bone has a fine internal structure that is not accurately reconstructed. The bone's internal structure resulted in significant diffraction. Consequently, the plane wave approximation employed in the T-ray CT reconstruction was not satisfied and the resolution was subsequently degraded.

Frequency Dependent Reconstruction

Time domain reconstructions of the sort shown in Figs. 4.63 and 4.67 are useful for revealing structural information, particularly if the internal structure of an object can be revealed. However, a more interesting problem is that of inferring functional information. Chapter 5 demonstrates classification techniques capable of utilising the frequency dependent information provided by THz imaging to differentiate between different tissue types (Ferguson et al. 2001c). The use of such algorithms with T-ray CT data promises to enable functional 3D imaging with T-rays.

Figure 4.68 shows an optical image of a vial containing a thin plastic tube. This target is used to demonstrate frequency-dependent 3D reconstruction. The target was imaged

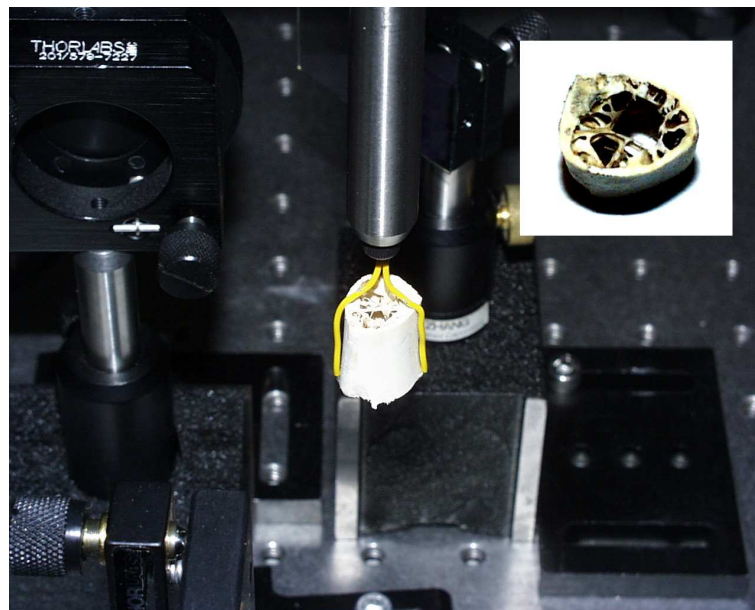


Figure 4.66. A section of turkey femur imaged with the T-ray CT system. The fine structure inside the bone is of the order of the THz wavelength and therefore causes difficulties in reconstruction.

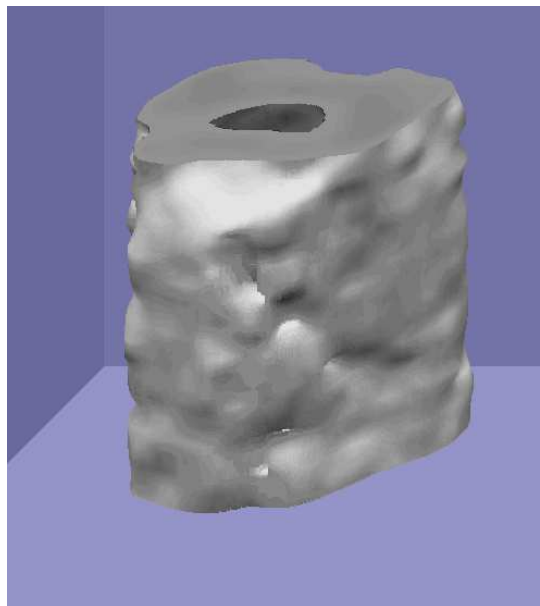


Figure 4.67. Reconstructed 3D image of a turkey femur. The turkey bone shown in Fig. 4.66 was imaged using the T-ray CT system, the reconstruction was performed and the 3D rendered image generated. The reconstruction used the amplitude of the THz pulses at each pixel to calculate the exponential absorption coefficient, ρ , as the input to the filtered backprojection algorithm.

4.6 T-ray Computed Tomography

with a 1 mm step size in the x and y dimensions, and at projections separated by 10° . First the reconstruction was performed using the timing of the peak of the THz pulse in the time domain to yield a reconstruction of the bulk refractive index. The reconstruction of the centre slice is shown in Fig. 4.69 and the 3D rendered image shown in Fig. 4.70 was produced by combining a number of the reconstructed slices. The iso-surface was constructed using the pixels where the reconstructed refractive index was 50% of the maximum index for the outer vial. The reconstructed image dimensions are quite accurate, the vial and cylinder diameters are within 15% of the actual dimensions measured with calipers. However, the vial thickness is much thicker than expected because of the coarse reconstruction grid size of 1.5 mm. The grid size may be improved using more projection angles.



Figure 4.68. A vial and plastic tube were used for testing the T-ray CT system. An optical image of the target.

T-ray CT has the potential to identify targets based on their frequency response in the far-infrared. Figure 4.71 shows the reconstruction of the vial sample using the data at 4 different frequencies. The resolution of the reconstruction improves as the frequency increases, however, the SNR decreases because most of the source power is at frequencies below 0.5 THz. Therefore the reconstructions at higher frequencies suffer from additional artifacts caused by noise.

The full frequency-dependent reconstruction algorithm described in Sec. 4.6.3 was then applied to the vial sample shown in Fig. 4.68. The central slice was reconstructed at each frequency. The pixels corresponding to the inner tube were averaged to yield the refractive index profile shown in Fig. 4.72. For reference the frequency dependent refractive index of the tube was calculated with normal THz-TDS and is also plotted. There is reasonable agreement between the two techniques although the result from

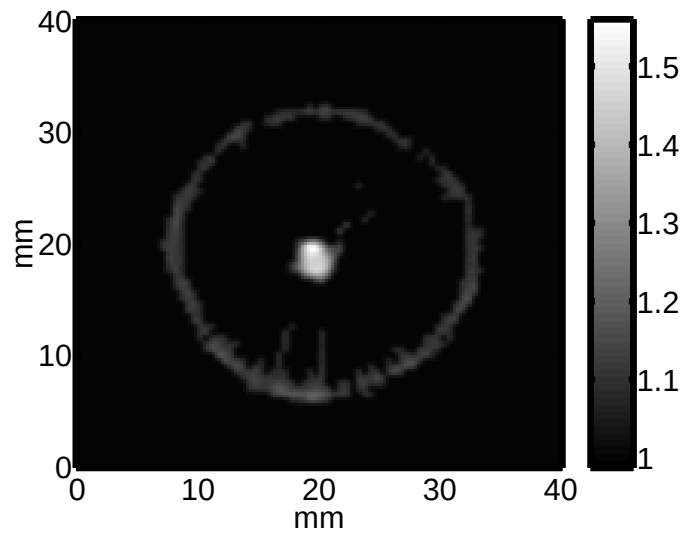


Figure 4.69. Reconstructed vial and plastic tube. The timing of the peak of the pulse in the time domain was used as the input to the filtered backprojection algorithm and the cross-section was reconstructed to yield the refractive index.

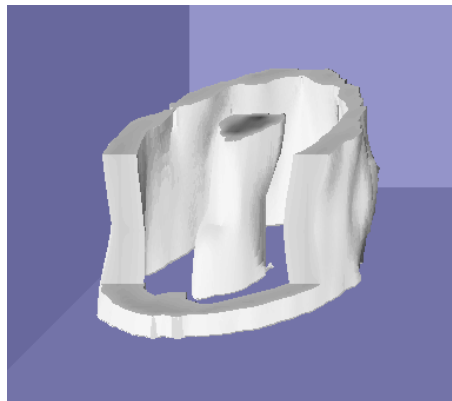


Figure 4.70. A 3D image of the reconstructed vial and plastic tube. Each cross-section was reconstructed using the timing of the peak of the pulse. The cross-sections were combined and a 3D surface rendered image produced. The surface was selected at 50% of the peak reconstructed refractive index. The front of the data has been cut away to allow the internal tube to be observed.

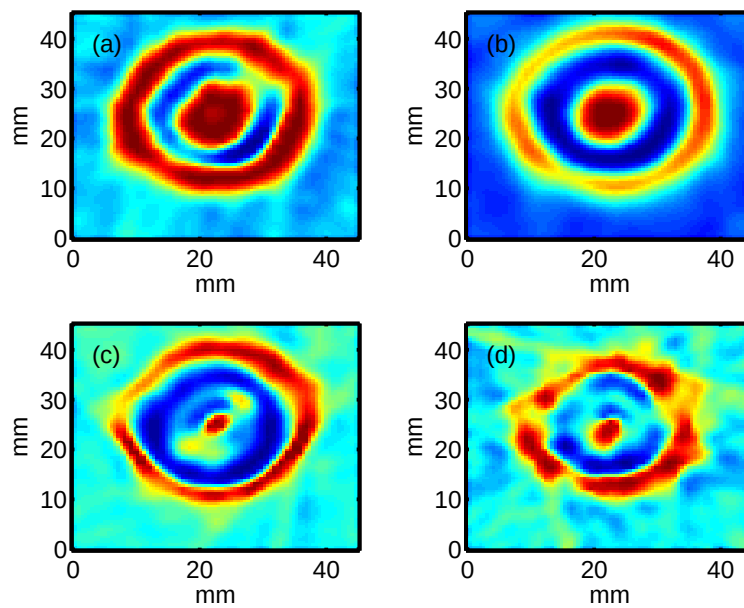


Figure 4.71. Frequency dependent reconstructions of the vial target. The measured data was Fourier transformed and the phase of the Fourier domain responses was used to reconstruct the sample at 4 different frequencies: (a) 0.2 THz, (b) 0.4 THz, (c) 0.6 THz, (d) 0.8 THz. The colour of each pixel maps the reconstructed refractive index. Red corresponds to the maximum index, followed by orange, yellow, green, blue, indigo and violet in order of decreasing refractive index.

T-ray CT is significantly noisier. This is primarily due to the disparate SNR of the two measurement techniques.

4.6.7 Amplitude vs Phase Reconstructions

For the polystyrene targets considered in Sec. 4.6.5 the absorption was not sufficient to allow a successful amplitude reconstruction because of the laser noise. By considering more highly absorbing targets this problem may be overcome. Figure 4.73 shows a hollow dielectric sphere made from celluloid. The sphere wall has a thickness of 0.4 mm, an absorption coefficient of 10.3 cm^{-1} and a refractive index of 1.62 at 0.5 THz. This target was imaged using the 3D T-ray CT system and both amplitude and phase reconstructions were performed in the time domain (Ferguson and Zhang 2002b, Ferguson et al. 2001b).

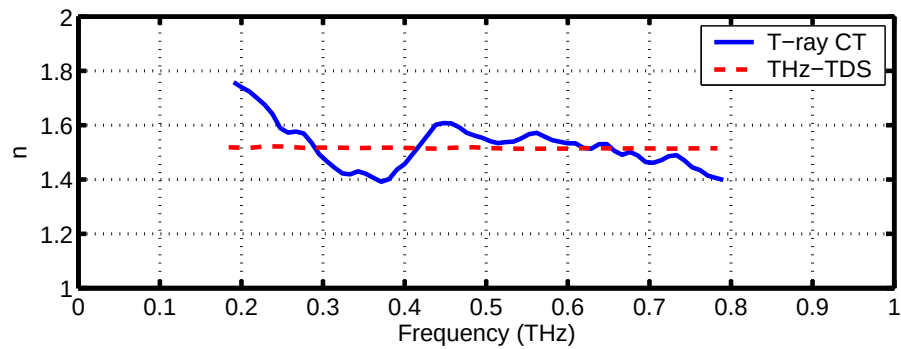


Figure 4.72. The frequency dependent refractive index of the plastic inner tube shown in Fig. 4.68. The refractive index was determined using T-ray CT, which required no assumptions regarding the sample thickness (solid line). The refractive index was also determined with standard THz-TDS using the measured thickness and the algorithm described in (Duvillaret et al. 1996) (dashed line). The noisiness of the T-ray CT response is due in part to the low SNR of the chirped probe pulse imaging method compared to THz-TDS.

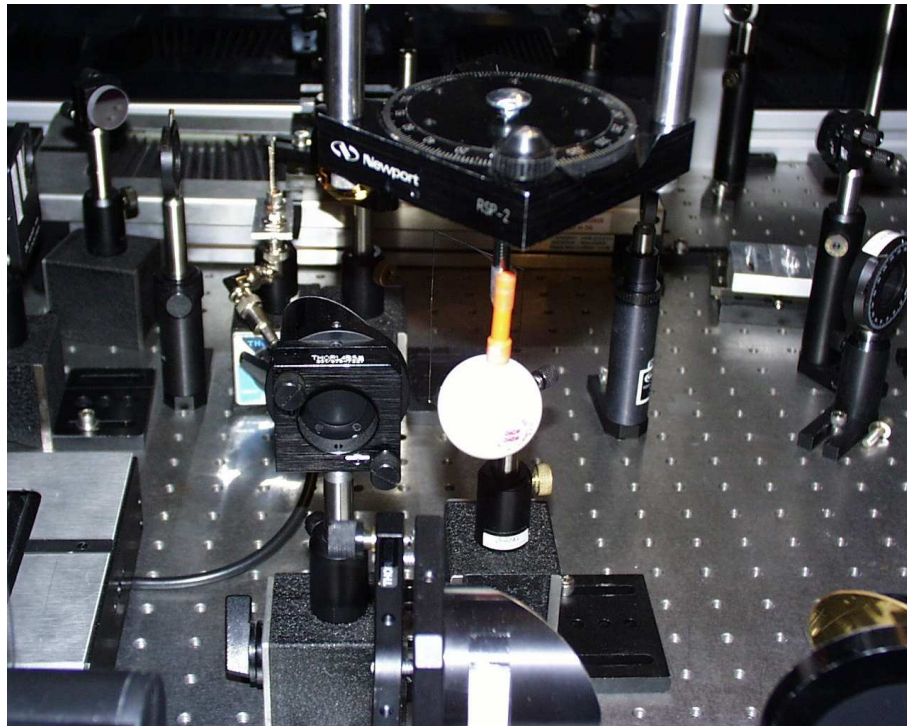


Figure 4.73. A hollow celluloid sphere imaged using T-ray CT. The celluloid sphere (ping pong ball) is attached to a plastic tube, which is rotated by the rotation stage. The sphere was scanned with a 1 mm step size and the THz image was obtained for 18 different projection angles.

4.6 T-ray Computed Tomography

Figures 4.74 and 4.75 show the reconstruction of several cross-sectional slices of the hollow celluloid sphere using the time domain ρ and τ based reconstructions respectively. The reconstructed thickness is 1.5 mm for Fig. 4.75 and almost 3 mm for Fig. 4.74, in comparison with the actual thickness of approximately 0.4 mm. There are several reasons for the reduced resolution. The Rytov approximation discussed in Sec. 4.5.1 imposes one limit on the resolution. In addition, a second limiting factor results from the reconstruction grid size. This grid size is largely determined by the image sampling resolution, which in turn is limited by the acceptable acquisition time. For a projection offset step size of 1 mm and 18 projection angles the minimum grid size is approximately 1 mm. However, neither of these limits explain the difference in resolution of the amplitude and phase based reconstructions. To address this question we reconsider the reconstruction algorithm and its implicit assumptions. The propagation model assumed in the reconstruction effectively neglects Fresnel loss. As will be shown shortly, this introduced a much more significant error in the amplitude of the THz pulses than the phase, and correspondingly degrades the ρ based reconstruction.

T-ray CT uses a focused beam of THz radiation with a focal spot of approximately 2 mm diameter. This beam is transmitted through the target and then detected using electro-optic sampling, providing both amplitude and phase information. A single detector is used to detect only the radiation transmitted straight through the target and not the scattered radiation. In practice parabolic mirrors are used to manipulate the THz beam and these collect the scattered radiation over a relatively small scattering angle ($< 10^\circ$).

As a result this technique is optimal for targets that do not result in significant scattering or refraction of the incident THz beam. Consider the target geometry illustrated in Fig. 4.76, consisting of multiple layers of different materials in air. Provided that the refractive index of the materials are small the THz beam direction will not be significantly altered ($> 10^\circ$) as it propagates through the target, and will still be detected.

If we further assume that the target is relatively smooth on the order of the THz spot size (2 mm) then the propagation equations for planar homogenous media apply. For a single planar slab the transmitted THz radiation, $u(\omega)$, at a frequency ω , is determined by the Fresnel transmission coefficients $t_{a,b}$ from material A to material B at each face of the slab and the plane wave propagation, $p_b(\omega, d)$, where:

$$t_{a,b}(\omega) = \frac{2\tilde{n}_a(\omega) \cos \theta}{\tilde{n}_a(\omega) \cos \beta + \tilde{n}_b(\omega) \cos \theta'}, \quad (4.112)$$

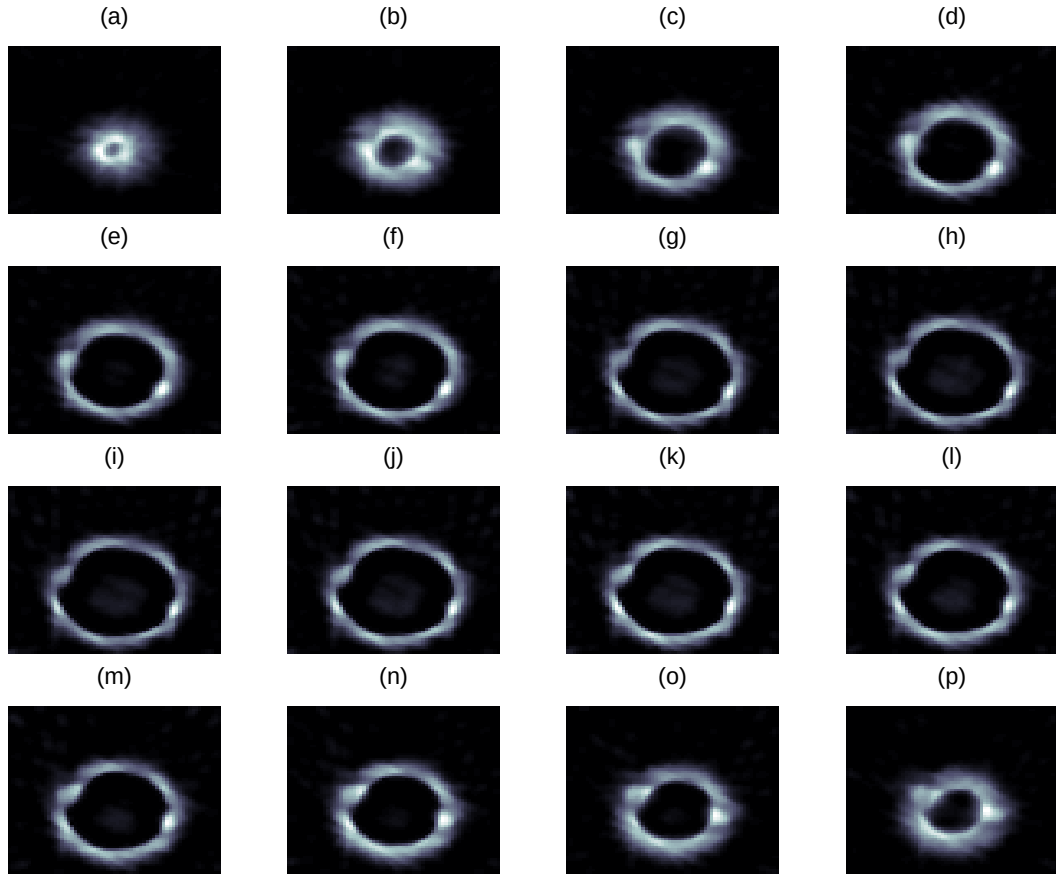


Figure 4.74. Reconstructed slices of the celluloid sphere using ρ . The peak of the time domain THz signals and a reference pulse were used to estimate ρ and the filtered backprojection algorithm was employed to reconstruct each horizontal cross-section of the target. Several slices through the sphere are shown, starting with the topmost slice. The reconstructed sphere wall thickness is approximately 3 mm.

$$p_b(\omega, d) = \exp\left(\frac{-i\tilde{n}_b(\omega)\omega d}{c}\right), \quad (4.113)$$

$\tilde{n}$ is the material's complex refractive index as a function of frequency, which is given by $\tilde{n}(\omega) = n(\omega) + i\kappa(\omega)$ where $n(\omega)$ is the real refractive index and $\kappa(\omega) = \alpha(\omega)c/(2\omega)$ is proportional to the absorption coefficient $\alpha(\omega)$. Here, c is the speed of light, θ is the angle of incidence, β is the angle of refraction governed by Snell's law and d is the length of the propagation path through the material.

For a general target consisting of multiple material interfaces i the transmitted radiation is given by:

$$u(\omega) = u_0(\omega) \prod_i t_{i-1,i}(\omega) p_i(\omega, d_i). \quad (4.114)$$

4.6 T-ray Computed Tomography

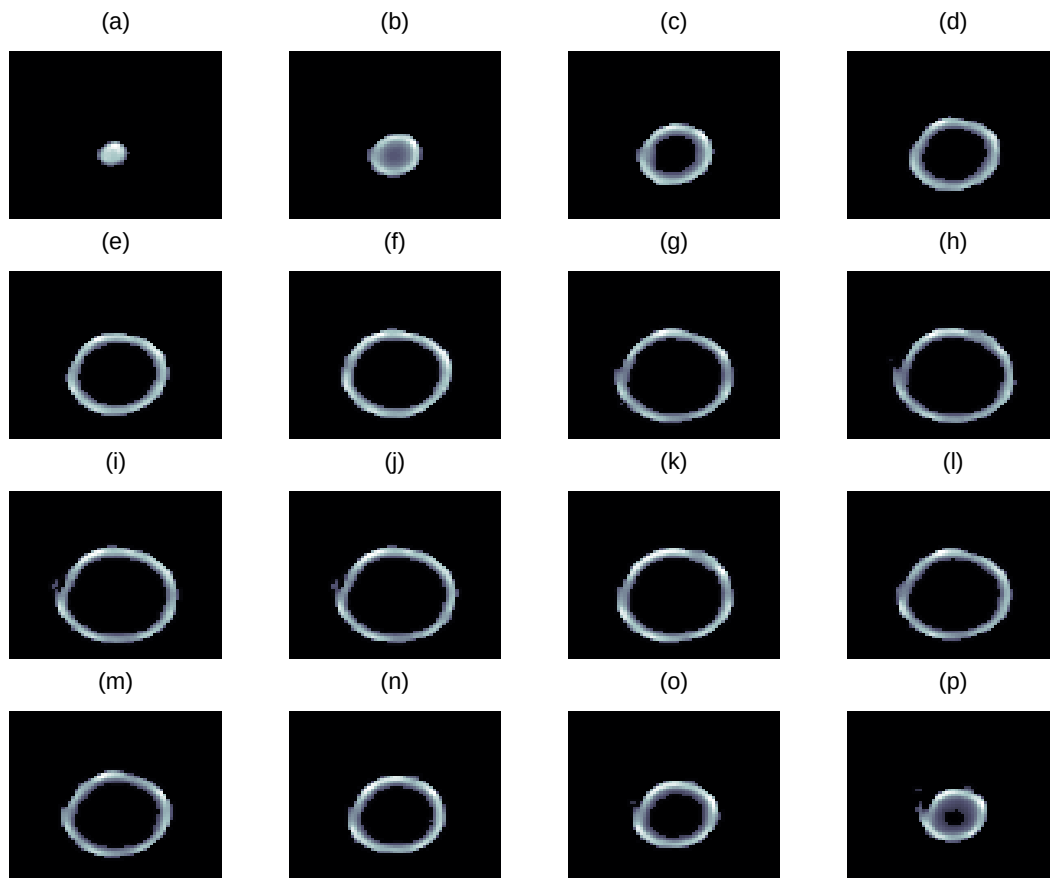


Figure 4.75. Reconstructed slices of the celluloid sphere using τ . The time domain THz signals were interpolated by a factor of 10 and cross-correlated with an interpolated reference pulse. The lag of the peak of the cross-correlation was used to estimate τ and the filtered backprojection algorithm applied. The reconstructed sphere wall thickness is approximately 1.5 mm.

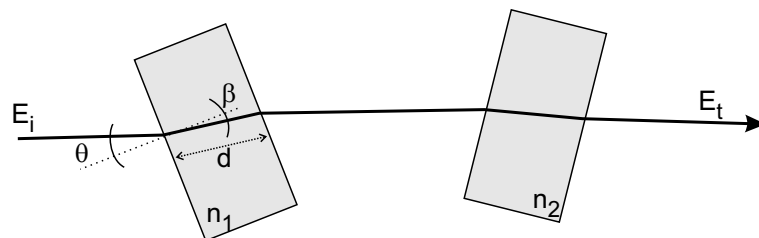


Figure 4.76. An example geometry for T-ray CT. The target consists of two materials with refractive index n_1 and n_2 .

By Fourier transforming the measured THz pulses we obtain the complex Fourier coefficients $u(\omega)$. If we consider the phase of the Fourier coefficients we find:

$$\arg [u(\omega)] = \arg [u_0(\omega)] + \arg \left[\prod_i t_{i-1,i}(\omega) \right] + \arg \left[\exp \left\{ \sum_i \left(\frac{-i\tilde{n}_b(\omega)\omega d_i}{c} \right) \right\} \right]. \quad (4.115)$$

For transmission tomography we are most interested in low absorption materials implying that $n(\omega) \gg \kappa(\omega)$, the second term in Eq. (4.115) is therefore negligible and Eq. (4.115) becomes:

$$\arg [u(\omega)] = \arg [u_0(\omega)] + \sum_i \left(\frac{-n_b(\omega)\omega d_i}{c} \right). \quad (4.116)$$

In the general case where there may be a large number of materials and d tends to 0, Eq. (4.116) becomes a line integral type equation where the measured phase is simply equal to the integral of the real refractive index of the target along the straight line between the emitter and the detector. This then allows us to employ the filtered back-projection algorithm to reconstruct the real refractive index as discussed in Sec. 4.6.3. The same analysis can be extended to the time domain where the timing τ of the pulses results in an accurate reconstruction as illustrated in Fig. 4.77 where the reconstructed cross-sections shown in Fig. 4.75 have been combined and surface rendered to produce a 3D image. The image is an isosurface at an amplitude of 50% of the peak reconstructed refractive index.

However, considering the amplitude of Eq. (4.114) yields

$$\|u(\omega)\| = \|u_0(\omega)\| \left\| \prod_i t_{i-1,i}(\omega) \right\| \left\| \exp \left\{ \sum_i \left(\frac{-i\tilde{n}_b(\omega)\omega d_i}{c} \right) \right\} \right\|. \quad (4.117)$$

For materials with $n \gg \kappa$ the second term of Eq. (4.117) cannot be safely neglected, without introducing errors in the reconstruction. For the targets considered in this section these errors manifest in a reduction in the resolution of the reconstruction.

This analysis reveals a number of additional conditions for the applicability of T-ray CT:

1. the sample should be smooth compared to both the wavelength of the radiation and the focal spot size,
2. the absorption coefficient of all materials in the target should be small compared to its refractive index,

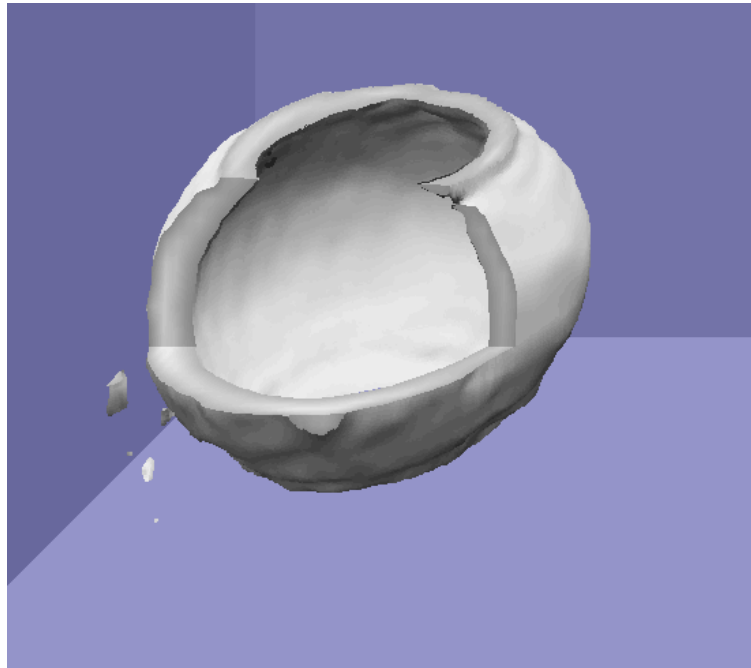


Figure 4.77. Reconstructed 3D image of a celluloid sphere. The timing τ of the time domain THz pulses was used as the input to the filtered backprojection algorithm. An isosurface at 50% of the peak reconstructed index is displayed.

3. the target's refractive index and geometry should not result in refraction of the THz beam beyond the collection optics.

4.7 Chapter Summary

This Chapter has described three novel T-ray tomography systems. These systems each have important advantages that lend them to specific applications. Applications of these techniques may include three-dimensional biological tomographic imaging, packaging/security inspection and industrial quality control. When combined with spectroscopic material identification algorithms, T-ray tomography systems may allow non-destructive signature detection of biological materials such as anthrax and TNT for mail, package and luggage screening.

4.7.1 T-ray Holography

T-ray holography utilises the temporal information available in coherent THz measurements with the windowed Fourier transform together with digital holographic techniques based on backpropagation of the Fresnel-Kirchhoff diffraction equation. This technique adds to the important field of 3D THz imaging to allow the 3D identification of point scatterers in a homogenous background media using THz-TDS measurements. Applications may include the identification of bubbles or fractures in manufactured components and security inspection. The technique provides the potential for real time 3D imaging and offers a resolution of under 1 mm in normal conditions. At longer wavelengths this technique may have biomedical applications such as breast cancer screening. Work is ongoing to extend the generality of the reconstruction algorithms.

4.7.2 T-ray DT

T-ray DT provides added capability by using linearised inverse scattering algorithms to invert the Helmholtz equation and determine the frequency dependent complex refractive index of the target. It can be performed relatively quickly by aid of 2D FSEOS THz imaging and allows wavelength limited resolution. The Born and Rytov approximations have been investigated using the T-ray DT system. The Rytov approximation was shown to impose less restrictive requirements on the target and result in a higher fidelity reconstruction. Much work has been performed inverting the wave equation for tomographic reconstruction in ultrasound and microwave fields without resorting to the first order approximations and it is expected that variations of these algorithms will prove fruitful for T-ray DT in the future. The T-ray DT system is only suitable for targets smaller than the THz sensor, which has a diameter of 2 cm. However, future systems may use a telescope arrangement of THz polyethylene lens to allow larger targets to be imaged. A further difficulty of T-ray DT is the low SNR caused by spreading the limited THz power (approximately 4 μ W average power) over the entire sensor area. T-ray DT systems will benefit greatly from higher power THz sources as they are developed.

4.7.3 T-ray CT

T-ray CT is a powerful technique due to its ability to extract the frequency dependent refractive index at each pixel of a 3D image. The focused THz beam allows a higher SNR to be achieved than either of the other techniques. However, this technique is very time consuming; a typical image of size 100×100 pixels measured at 18 projection angles can take over an hour. Currently, CCDs with MHz sample rates and 12 bit sensitivity are not available but as this technology becomes common the T-ray CT acquisition time can be reduced appreciably. The T-ray CT reconstruction algorithm imposes a number of restrictions on the target. T-ray CT works well for targets with features that are large relative to the wavelength of the THz radiation (0.3 mm at 1 THz), however for more complex targets with fine structure the filtered backprojection algorithm is unable to accurately reconstruct the target because diffraction effects dominate the measurements. The focal width and depth of the T-ray beam are also important parameters that impact on the resolution and accuracy of T-ray CT.

T-ray CT is a notable extension of THz time-domain spectroscopy with several potential applications. T-ray CT has been used to extract the frequency dependent refractive index of a 3D target thereby providing spectroscopic images of weakly scattering objects. T-ray CT provides the refractive index of the sample without requiring *a priori* knowledge of the sample thickness and allows the internal structure of objects to be revealed. The frequency dependent reconstruction is noisier than techniques that neglect dispersion and implicitly average the frequency domain data. However, as the SNR of the T-ray CT hardware is improved it is anticipated that the frequency dependent information will yield important functional information and enable material classification by this method.

4.7.4 Looking Forward

This Chapter has demonstrated practical 3D THz imaging techniques. These techniques provide the capability to reconstruct spectroscopic 3D images of targets. The full potential of 3D THz imaging will be realised when it is coupled with powerful signal classification algorithms to allow material identification based on the reconstructed 3D images. The combination of 3D THz imaging and classification algorithms, will allow the identification of materials inside optically opaque objects, for example, the detection of anthrax beneath layers of packaging.

Consequently, in the next Chapter, we develop the groundwork for this vision, by investigating algorithms for the classification of materials based on 2D T-ray imaging data. This is an essential first step towards the future goal of developing 3D THz classification algorithms, which remains an important open question for future research.

Chapter 5

Material Identification Using THz Imaging

THE ultimate goal in all terahertz systems is to extract information about the sample under test. For example, this information may be the frequency dependent index of refraction for a semiconductor wafer or the resonant absorption frequencies for gas sensing. For inspection imaging applications we desire to detect and differentiate between different materials based on the THz response.

In this Chapter a classification architecture is developed. Emphasis is placed on the problem of feature extraction to reduce the complex THz spectral responses to several features allowing simple classification of different materials. Three case studies are performed to demonstrate the potential of the classification framework and the power of THz spectroscopy. The identification of specific materials was investigated in the following application settings:

1. biological tissue type classification,
 2. detection of bacterial spores inside envelopes, and differentiation from other powders, and
 3. *in-vitro* differentiation of cancerous and normal human cells.
-

"Knowledge is the small part of ignorance that we arrange and classify."

- Ambrose Bierce

5.1 Introduction

The field of signal processing techniques for terahertz systems is relatively unexplored, however work has been reported in determining optimal techniques for denoising (Ferguson and Abbott 2000, Ferguson and Abbott 2001b), extracting material constants (Duvillaret et al. 1999, Dorney et al. 2001a), gas mixture analysis (Mittleman et al. 1998a, Mouret et al. 1999) and material classification (Hadjiloucas et al. 2002a). An intriguing application of THz signal processing used a metallic transmission grating to differentiate a time domain THz pulse in accordance with classical diffraction theory (Filin et al. 2001). This Thesis adds to this important field by developing a classification framework tailored to process the measured THz spectra with a goal of identifying different materials using their terahertz responses. This has particular application in a medical imaging setting where extracted diagnostic information is required to aid the medical practitioner in assessing a patient.

5.1.1 Pattern Recognition

The origins of the field of classification or pattern recognition can be traced as far back as the ancient philosopher Plato who defined a 'pattern' as the ideal form, or the essential properties of a class of objects as distinct from accidental or random properties that vary between objects in a class (Bloom 1991). Watanabe (1985) defines a pattern as

"...opposite of a chaos; it is an entity, vaguely defined, that could be given a name."

The modern mathematical field of pattern recognition owes much to Bayesian decision theory (Bayes 1763, Laplace 1812) and now encompasses an immense body of knowledge and has application within practically every scientific discipline (Duda 2001).

Simply stated the problem of pattern recognition or classification is that of taking raw data and assigning that data to one of several potential classes. This principle is crucial to our survival and is one of the prime roles of the human brain. In fact, Nobel laureate and one of the founding fathers of artificial intelligence, Herbert Simon, concluded

Table 5.1. Examples of pattern recognition applications. The field of pattern recognition has application in almost every scientific discipline. Several examples are provided here. In each case the input pattern, or the raw data to be processed, is identified as well as the desired output or the classification classes. Reproduced from (Jain et al. 2000).

Problem Domain	Input Pattern	Pattern Classes
Bioinformatics	DNA sequence	Known genes/patterns
Data mining	Points in n -dimensional space	Compact, separated clusters
Document image analysis	Image of a document	Alphanumeric characters
Industrial automation	Intensity or range image	Defective/non-defective
Multimedia database retrieval	Video clip	Video genres
Biometric recognition	Face, iris, fingerprint	Authorised users
Speech recognition	Speech waveform	Spoken words

that pattern recognition is central in almost all human decision making tasks (Simon 1996). As a result, a field of research has arisen attempting to replicate the processing of the brain in artificial neural networks (ANN). Principle examples of classification tasks include speech recognition, target identification in images and DNA sequence identification. Table 5.1 provides an overview of the scope of applications of pattern recognition (Jain et al. 2000).

The pattern recognition task can be conceptually divided as shown in Fig. 5.1. The pre-processing stage typically involves denoising the data and tasks such as normalisation or correction for ambient lighting conditions in image processing tasks. In our case the preprocessing stages investigated include wavelet denoising to remove noise from the THz time domain pulses, and deconvolution, which isolates the influence of the material from that of the ambient system and environment. These techniques are the focus of Sec. 5.2.

Feature extraction is a critical step in the pattern recognition process. The quality of the feature extraction methods can render the classification task either trivial or futile. Ideally features should be chosen such that there is a small intraclass variation and a large interclass variation. A related problem to feature extraction is that of feature selection. In theory an infinite number of features are available, and a subset of these must be chosen to implement a feasible classifier. How should the features be chosen? How *many* should be chosen? These questions and others are addressed in Sec. 5.3 where several schemes for feature extraction and selection are introduced.

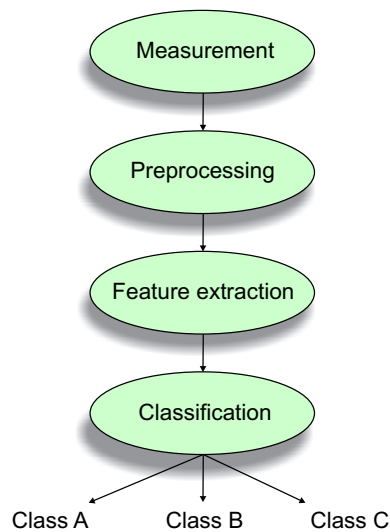


Figure 5.1. Conceptual segmentation of the pattern recognition problem. The raw data is measured and the goal of pattern recognition is to assign the data to one of several potential classes. The data is often preprocessed to remove noise from the measurement and simplify subsequent processing without discarding information. The feature extraction operation calculates the value of certain features or properties of the data. This serves to reduce the size of the data set that is then passed to the classifier. The classifier evaluates the feature data according to knowledge of the properties of each potential class.

Finally, the features must be evaluated and classified as belonging to one of several potential classes. Before this is possible the classifier must be trained with knowledge about the potential classes. There is, therefore, a parallel process to that described in Fig. 5.1. In this parallel process the response of known targets belonging to each of the available classes are measured, the data preprocessed and features extracted. These features are used to train the classifier. In some applications, such as data mining, the training step may be omitted and *unsupervised* classification performed (Duda 2001). In this Thesis, training data was readily obtainable, supervised classification was therefore preferred as it generally offers improved performance (Duda 2001).

A vast amount of research has been conducted into classification algorithms of varying complexity and sophistication. In this Thesis an emphasis was placed on feature extraction methods as these provide a model of the underlying pattern and may often allow physical characteristics of the targets to be inferred. Many classification algorithms result in complex decision boundaries thereby abstracting over the power of

the features themselves to differentiate between classes. In this work a simple Mahalanobis distance classifier was used, as described in Sec. 5.5.

5.1.2 THz Classification

The submillimetre spectroscopic measurements obtained from T-ray systems contain a wealth of information about the sample under test. The use of THz spectroscopy for material identification has received attention in a number of different application settings (Chamberlain et al. 2002). It has been demonstrated for gas concentration determination (Mittleman et al. 1998a, Jacobsen et al. 1996, van-der-Weide et al. 2000), leaf moisture content analysis (Hadjiloucas et al. 1999, Hadjiloucas et al. 2002a), and cancer detection (Woodward et al. 2002, Woodward et al. 2003).

In several cases, most notably for gas spectroscopy, the THz response exhibits sharp resonant lines and the amplitude of these resonances may be used to enable classification. Mittleman et al. (1998a) used an all pole filter to fit to these resonant peaks and used the filter coefficients as classification features. For solid spectroscopy alternate methods have been investigated. The Karhunen-Loève transform has been applied to the THz responses for feature extraction to maximise the Euclidean distance between classes of leaves in different stages of drought (Hadjiloucas et al. 2002a). Time domain metrics based on the deconvolved THz responses have also shown promise in differentiating between the responses of cancerous and normal dermal tissue (Woodward et al. 2002).

An important potential application for THz inspection systems is in the detection and identification of illicit materials including drugs and explosives. Watanabe et al. (2004) have demonstrated component system identification algorithms for the detection of methamphetamine (a commonly abused substance in Japan) and an aspirin reference (Kawase et al. 2003a). Oliveira et al. (2003) have conducted promising studies into the use of neural network classification algorithms in enabling THz detection of concealed cyclotrimethylene-trinitramine (RDX) explosives and bioagents. All-electronic THz systems have been used for the characterisation of explosive and biological hazards, and show potential for standoff sensing-at-a-distance (Choi et al. 2004).

Wavelet techniques have also been recently investigated for material identification using THz imaging data. Wide-band cross ambiguity functions were used to extract features, which allowed classification of nylon and resin phantoms (Handley et al. 2004).

5.2 Preprocessing

Signal processing techniques may be used to improve the speed, resolution and noise robustness of T-ray imaging systems. This section considers a number of signal processing techniques suitable for denoising and extracting information from the data obtained in a terahertz pulse imaging system. Two main preprocessing techniques are emphasised: wavelet denoising and Wiener deconvolution. These preprocessing stages are important facets of the pattern recognition framework, as the removal of noise prior to feature extraction can significantly improve classification performance.

There are several sources of noise in terahertz systems, due to both systematic and random errors. One method to reduce random errors due to noise is to average subsequent measurements for the same sample, however this increases the time required to perform the measurement. Signal processing potentially offers an improved solution to the noise problem.

Wavelets are of critical interest in this research as they possess a range of extremely attractive properties for this application. This section includes an evaluation of the quality of wavelet denoising of terahertz waveforms and a comparison of the different wavelet bases in THz denoising.

Another significant source of errors and ambiguity in THz systems is the system hardware itself. The signal obtained for a sample is a result of the far-infrared properties of the sample (which are of critical interest) and the properties and non-idealities of the system itself – these include electrical and optical reflections from system components and numerous other effects (Mittleman et al. 1998a). In order to accurately classify the THz spectra it is vital that the sample signal characteristics be isolated from the system characteristics. This is generally performed by the process of deconvolution. The standard deconvolution process is extremely sensitive to noise and can result in considerable errors when noise is present. Improved methods of deconvolution can optimally deconvolve noisy signals (Mittleman et al. 1998a).

The major goal of most experiments involves the determination of the complex, frequency-dependent refractive index of the substance under test. In the vast majority of cases this has been calculated using the following simple procedure. The time-domain THz pulse is measured using the system shown in Fig. 1.2 without a sample in place. This signal is referred to as the system response. The sample is then added to the system and the terahertz pulse measured again. The Fourier transforms of these two

signals are found and then the ratio of the transforms yields the complex transmission coefficient of the sample as a function of frequency (Duvillaret et al. 1996, Duvillaret et al. 1999). Taking the ratio in the frequency domain performs the deconvolution of the signal and serves to isolate the sample dependent characteristics. Subsequent processing is then application dependent. For dielectric and semiconductor characterisation the refractive index can be derived from the transmission coefficients (Jiang et al. 2000a), as detailed in Appendix C, whereas for gas sensing applications the transmission frequency response is analysed to identify absorption spectra corresponding to specific molecular resonances. Signal processing techniques such as linear predictive coding (LPC) have been employed to improve the sensitivity in gas sensing and chemical recognition applications (Mittleman et al. 1998a, Jacobsen et al. 1996).

One of the significant problems posed by the above processing is the inherent noisiness of the deconvolution process. The simple ratio deconvolution amplifies any high frequency noise in the signal (Castleman 1996). One method of countering this problem is through the application of a pre-processing filter. Wavelet denoising filters have been suggested due to their pulse-like nature (Mittleman et al. 1998a, Micken et al. 2000). Another approach to this problem is the Wiener filter (Mittleman et al. 1998a) that performs system deconvolution and also performs optimal noise cancellation in the mean-square error sense.

There are a large number of noise sources in terahertz systems. The relative intensity of these sources varies depending upon the particular setup and sample under test, but it is generally found that the emitter noise dominates all other noise contributions. This noise is a result of random intensity fluctuations in the ultrafast laser and has been quite extensively studied (Haus and Mecozzi 1993, Poppe et al. 1998). Other major sources of random error are Johnson and shot noise in the THz detector (Duvillaret et al. 2000) as well as thermal background radiation in the THz regime. The coherent nature of T-ray systems allow them to achieve impressive performance despite very high relative noise magnitudes. The noise is incoherent and adds randomly for successive optical pulses while the signal is coherent and scales linearly with the number of gating pulses (van Exter and Grischkowsky 1990b).

A lock-in amplifier may be used to digitise the signal and provides a significant improvement in signal to noise ratio. In one typical example the LIA provided an increase in SNR of up to 100 times at the expense of acquisition speed (Mittleman et al. 1996).

5.2 Preprocessing

Figure 5.2 shows the effect of the LIA time constant on the measurement noise by presenting a THz response measured with two different time constants. The improvement in SNR with increasing LIA time constant is evident.

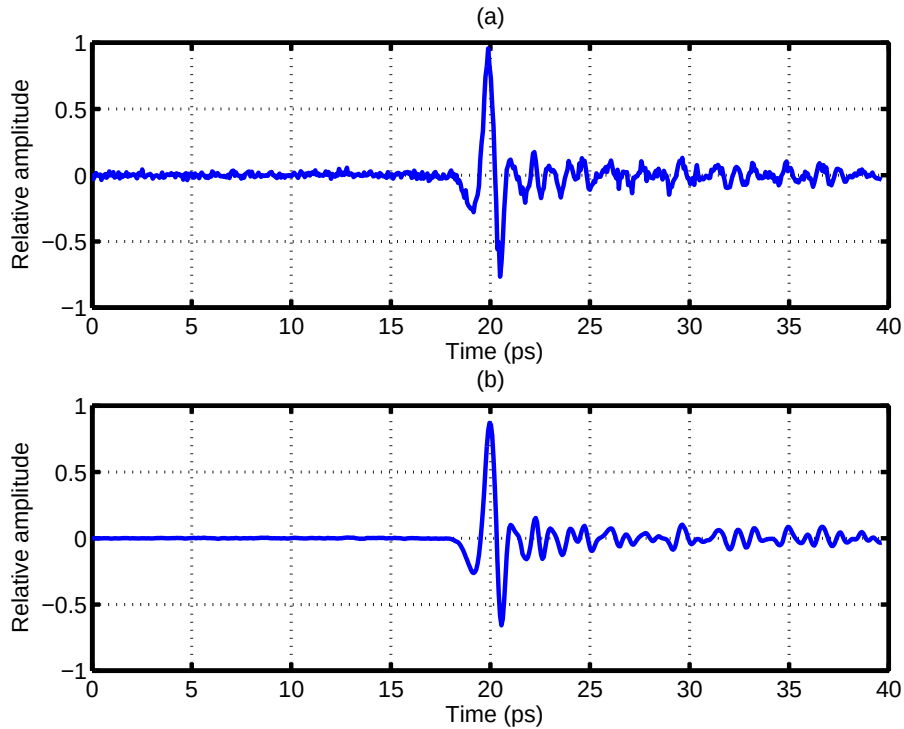


Figure 5.2. Terahertz responses measured with differing LIA time constants. (a) THz pulse measured with a short time constant of 1 ms. (b) The same response measured with a time constant of 100 ms.

In addition to these random errors there are several potential systematic errors in the system. These include parasitic reflections of the THz beam from system components, phase errors due to delay line misalignment and absorption and dispersion of water vapour (van Exter et al. 1989).

To investigate the relative benefits of different signal processing methods a standard set of T-ray data was used. It consisted of a 100×100 pixel image of an oak leaf with an insect on the left side of the leaf as shown in Ch. 3 (Fig. 3.12). The image has a spatial resolution of approximately 1 mm. For each pixel the time response of the terahertz pulse was recorded over 12 ps (10^{-12} s) at an effective sample rate of 25 terasamples/second. Examples of these responses for each of the three distinct media (leaf, insect and free air) were shown in Fig. 3.11.

5.2.1 Definitions and Notation

The signals considered here, $f(k), k \in 0..N-1$, are real-valued, finite, discrete-time functions defined on the set of real numbers $\mathbb{R}$, where N is the number of samples.

The inner product of two sequences f and g is written

$$\langle f, g \rangle = \sum_{k=0}^{N-1} f(k) g(k). \quad (5.1)$$

The dyadic, discrete wavelet transform of a sequence f with respect to the mother wavelet ψ as a function of scale, m , and offset, n , is given by (Meyer 1993)

$$\begin{aligned} d_i = W_\psi f(m, n) &= \frac{1}{\sqrt{2^m}} \sum_{k=0}^{N-1} f(k) \psi \left(\frac{k - n2^m}{2^m} \right), \\ &= \langle f, \psi_{m,n} \rangle. \end{aligned} \quad (5.2)$$

The Fourier transform of a sequence $f(k)$ is denoted by $F(\omega)$ and is given by

$$F(\omega) = \sum_{k=0}^{N-1} f(k) e^{-i\omega k}. \quad (5.3)$$

The discrete convolution between two sequences f and g is the sequence $f * g$ given by

$$(f * g)(l) = \sum_{k=0}^{N-1} f(k) g(l - k). \quad (5.4)$$

5.2.2 Problem Definition

We consider the problem of determining the complex, frequency-dependent transmission coefficients for a given sample, whether that be a gas, a semiconductor or biological tissue. Figure 5.3 illustrates the system and signals we are considering.

Let $x_i(k)$ be the measured THz response for pixel, i , in free space,

$$x_i(k) = f(k) + n_i(k), \quad k = 0, \dots, N-1, \quad (5.5)$$

where $f(k)$ is the input signal generated by the terahertz emitter and $n_i(k)$ is Gaussian white noise.

Similarly, let $y_j(k)$ be the terahertz response obtained for pixel, j , containing the sample under test

$$y_j(k) = g(k) + n_j(k), \quad k = 0, \dots, N-1, \quad (5.6)$$

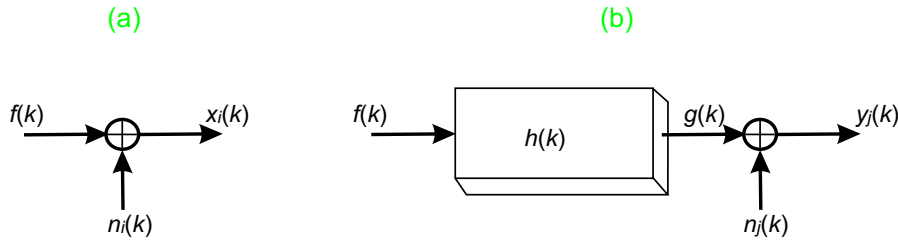


Figure 5.3. Block diagram of the elements used to define the problem. (a) The case where the sample is not present. (b) The case when the sample is included.

where $g(k)$ is the output of the unknown system when $f(k)$ is applied and $n_j(k)$ is Gaussian white noise. We model the response of the sample as a linear, time-invariant system:

$$g(k) = f(k) * h(k), \quad (5.7)$$

$$y_j(k) = f(k) * h(k) + n_j(k), \quad (5.8)$$

$$= [x_i(k) - n_i(k)] * h(k) + n_j(k), \quad (5.9)$$

where $h(k)$ is the impulse response of the sample under test.

The goal then is to design an algorithm to optimally (in the mean square error sense) determine $h(k)$ and $H(\omega)$ for the sample, given the noisy measured signals $x(k)$ and $y(k)$. It should be noted that this analysis is a simplification of the problem to aid tractability. In practice the measured sample response is determined by the potentially non-linear responses of the sample, the THz emitter and the detector.

5.2.3 Wavelet Denoising

General Wavelet Theory

If $f(k)$ and $g(k)$ can be accurately estimated from the noisy observations the problem can be simply solved from Eq. (5.7). Wavelet denoising represents a promising method in this regard. The theory of the wavelet transform has existed for many years in a number of forms. In the late 1980's Stéphane Mallat unified the various theories and coined the term: 'the Wavelet Representation' (Mallat 1989). Since then wavelets have found application in a wide range of fields as a result of their attractive and efficient properties.

Discrete wavelet methods are extremely efficient and computationally inexpensive. The fast discrete wavelet transform (DWT) allows wavelet coefficients to be calculated with a computational complexity of $\mathcal{O}(N)$, as compared with $\mathcal{O}(N \log N)$ for the DFT.

Wavelets have been shown to be particularly useful in the analysis of non-stationary signals and in image processing. This is because the wavelets, which form the basis functions for the transform, are localised in both time (or space) and frequency (or spatial frequency). This is in contrast to the Fourier transform, which uses infinite sinusoids as the basis functions.

The time-frequency localisation of the wavelet basis functions make the wavelet transform a more efficient representation of pulsed functions such as THz pulses. This allows for more effective denoising, compression and statistical estimation than Fourier analysis. In fact, it has been shown that wavelet bases are optimal for representing functions containing singularities (Donoho 1993). The goal of the wavelet transform in our context is to allow the measured signal to be separated into coherent structure and incoherent noise.

Wavelet shrinkage denoising is widely used for this purpose. Donoho (1995) defined the process of soft thresholding in the wavelet domain and proved that it was optimal in the mean square error sense. Soft thresholding is performed via the following procedure:

1. Determine the wavelet coefficients, d_i , by taking the wavelet transform (Equation 5.2).
2. Calculate the threshold value, T ,

$$T = \sigma \sqrt{2 \log_e N}, \quad (5.10)$$

where σ is the noise level and N is the number of samples.

3. Threshold the wavelet coefficients by moving them all towards zero by the threshold amount,

$$d_i = \begin{cases} d_i - T & \text{if } d_i \geq T, \\ d_i + T & \text{if } d_i \leq -T, \\ 0 & \text{if } |d_i| < T. \end{cases} \quad (5.11)$$

4. Perform the inverse wavelet transform to recover a time domain signal.

5.2 Preprocessing

More advanced algorithms have been proposed for denoising and signal analysis. These include wavelet packets (Chui 1992), the matching pursuit algorithm (Mallat and Zhang 1993) and many others. However, this study focuses solely on the simple denoising procedure outlined above.

Mittleman et al. (1998a) first suggested the use of the wavelet transform for THz processing and showed that the wavelet transform is an efficient representation of THz pulses. We examine this idea in detail and quantify the benefits offered by the wavelet denoising technique. A number of other authors have demonstrated wavelet denoising of THz data. Hadjiloucas et al. (2003) developed a method for optimising the compressional ability of the wavelet basis for a given THz pulse by parameterising a wavelet transform filter in terms of finite impulse response (FIR) filter coefficients (Sherlock and Monro 1998). An unconstrained optimisation algorithm was used to determine the filter coefficients to maximise an objective function defined by the energy retained by the thresholded wavelet coefficients. This method was used to preprocess the THz responses used to characterise THz waveguides, which is an important focus of recent research (Hadjiloucas et al. 2002b, Hadjiloucas et al. 2003, Sabetfakhri and Katehi 1994, Collins et al. 1999, McGowan et al. 1999, Gallot et al. 2000). The wavelet transform has also found application in optimising the integration time for Fourier transform infrared spectroscopy (FTIR) (Galvão et al. 2002), and the wavelet coefficients may be used for classification of the THz FTIR spectroscopy responses (Galvão et al. 2003).

The discrete wavelet transform may also be used to compress THz image data for efficient storage of biomedical images (Handley et al. 2002). It has been shown that THz time series can be compressed to 20% of its initial size without causing significant degradation of the extracted refractive index information.

Choosing a Wavelet Family

A large number of wavelet bases have been developed for different applications. Some examples of these wavelets are shown in Fig. 5.4. The leaf T-ray response is decomposed using the example wavelet bases and the wavelet coefficients are shown in Fig. 5.5. These wavelet bases each exhibit different properties and the following discussion addresses the question of determining the ideal mother wavelet for representing and denoising the T-ray data shown in Fig. 3.11.

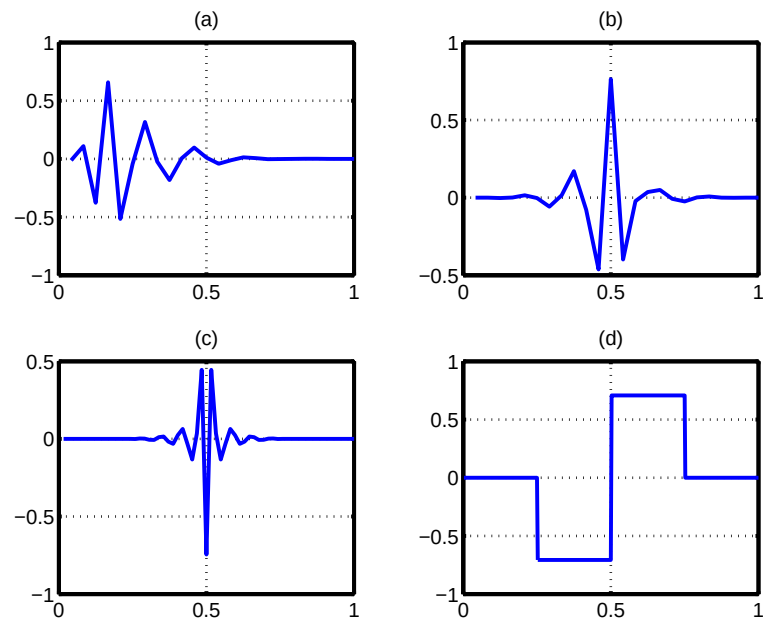


Figure 5.4. Examples of different wavelet basis functions, ψ . (a) Daubechies order 12, (b) Symlet order 12, (c) Meyer, and (d) Haar (Daubechies order 1).

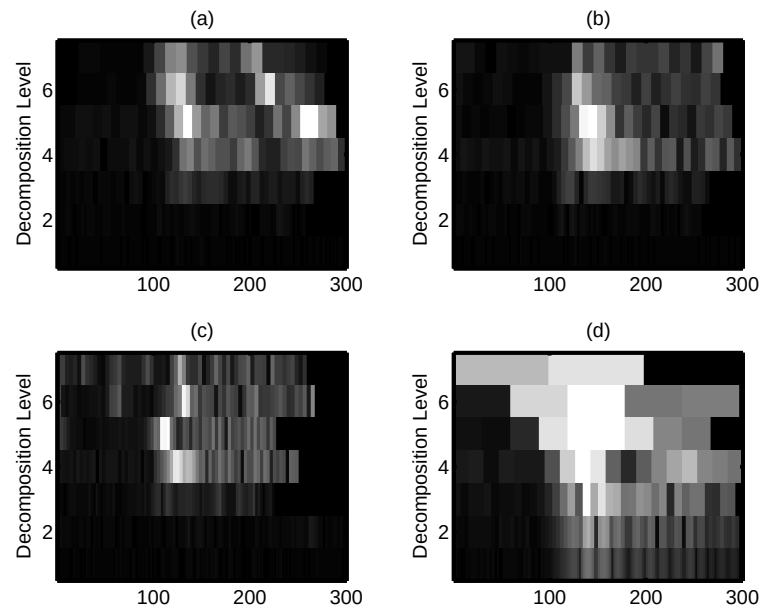


Figure 5.5. Wavelet coefficients for a T-ray response using different wavelet basis functions. (a) Daubechies order 12, (b) Symlet order 12, (c) Meyer, and (d) Haar (Daubechies order 1). The vertical axis shows the decomposition level or scale of the wavelet, while the horizontal axis depicts the time in units of samples. The greyscale intensity is proportional to the amplitude of the wavelet coefficients.

The goal of wavelet denoising is to approximate the noiseless function with as few non-zero wavelet coefficients as possible. The wavelet family associated with wavelet ψ should therefore be chosen to produce a maximum number of wavelet coefficients that are close to zero. The main properties of the wavelet that will affect this are its regularity, the number of vanishing moments and the compactness of its support (Mallat 1999).

A wavelet ψ has p vanishing moments if

$$\int_{-\infty}^{+\infty} t^k \psi(t) dt = 0 \quad \text{for } 0 \leq k < p. \quad (5.12)$$

Thus ψ is orthogonal to any polynomial of degree $p - 1$. If the signal to be transformed, f , is regular and can be approximated over a small interval by a Taylor polynomial of degree k and if $k < p$, then the wavelet is orthogonal to this polynomial and wavelet coefficients will be small for fine scales (high-resolution), thus for smooth functions a wavelet with a higher number of vanishing moments will represent the function with fewer large coefficients.

The size of support of a wavelet ψ refers to the range over which ψ has non-zero values, that is, it is a measure of the temporal localisation of the wavelet. The wider the support of the wavelet the more large amplitude coefficients are generated by peaks in the input signal f . This is a particular problem if the signal has many isolated singularities.

To reduce the number of large amplitude coefficients we must reduce the support size and increase the number of vanishing moments of ψ . However, it can be shown (Mallat 1999) that if ψ has p vanishing moments then its support is at least $2p - 1$. Therefore some trade off must be made. Daubechies wavelets are optimal in this regard as they offer the minimum support for a given number of vanishing moments (Daubechies 1992).

The regularity of ψ has a limited effect on thresholding efficiency. Its main importance is in the field of image processing where irregular wavelets can result in obvious discontinuous artifacts in the processed image. Other properties that distinguish between wavelets are their symmetry and orthogonality.

We limit this investigation to orthogonal, dyadic wavelet transforms due to the very fast algorithms available for their calculation, however many applications such as

speech processing require non-dyadic wavelet processing to accurately represent subtle changes in scale and delay (Young 1993). Non-dyadic wavelet processing techniques, such as the Over-Complete Wavelet Transform (Mallat 1999), represent an open area for future research.

Experimental Determination of the Optimal Wavelet

Experiments were performed to determine which wavelet performed best in denoising noisy T-ray data. Three typical THz pulses were considered corresponding to a pixel within each of the distinct media shown in Fig. 3.12, the free air, the oak leaf and the insect. The following experimental procedure was then adopted:

1. White, Gaussian noise was added to the THz pulses such that the signal to noise ratio (SNR) was 3 dB.
2. The soft wavelet denoising procedure described in Sec. 5.2.3 was applied to the noisy pulse using a given wavelet, ψ .
3. The resultant SNR was measured by comparing the denoised pulse with the original pulse. The SNR was calculated using the following formula,

$$\text{SNR(dB)} = 10 \log \left(\frac{\sum_{k=0}^{N-1} a(k)^2}{\sum_{k=0}^{N-1} [a(k) - b(k)]^2} \right), \quad (5.13)$$

where $a(k)$ was the original terahertz signal and $b(k)$ was the final signal after noise has been added and wavelet denoising performed.

4. This procedure was repeated 100 times to consider multiple realisations of the noise. The resultant SNR values were averaged to yield the average SNR for the given wavelet, ψ .

This procedure was then repeated using Daubechies, Meyer, Symlet and Coiflet wavelets. Within each wavelet family, varying wavelet orders were also tested. The order of the wavelet, M , is of particular concern to this discussion as it determines both the number of vanishing moments and the support length for the wavelet. Table 5.2 shows the properties of the wavelets considered here. More details on the wavelet properties can be found in the literature (Mallat 1999, Daubechies 1992).

5.2 Preprocessing

Table 5.2. Comparison of the major properties of wavelet bases. Here, M signifies the order of the wavelet.

Characteristic	Wavelet			
	Meyer	Daubechies	Coiflet	Symlet
Regularity	infinite	low, $\propto M$	$\propto M$	$\propto M$
Support Length	infinite	$2M - 1$	$6M - 1$	$2M - 1$
Symmetric	yes	no	nearly	nearly
# of Vanishing Moments	0	M	$2M$	M
Orthogonal	yes	yes	yes	yes

Table 5.3. SNR of T-ray pulses after wavelet denoising. White noise was added to the original signals such that the SNR was 3 dB before the denoising process was applied. The signals were denoised 100 times to average of different noise realisations. This process was conducted for each of the major wavelet families of varying order.

Wavelet Family	Order (M)	denoised SNR (dB)		
		Free Air	Leaf	Insect
Daubechies	1	8.4	7.9	10.1
	5	11.2	11.9	13.3
	10	11.6	11.0	12.1
	15	10.8	10.5	10.8
	20	10.4	10.4	12.1
	25	9.5	8.4	11.3
Coiflet	1	10.6	10.5	11.5
	2	11.7	11.4	11.4
	3	12.0	11.7	11.4
	4	12.5	12.1	13.3
	5	12.0	12.1	12.4
Symlet	1	9.1	8.3	10.0
	5	10.9	11.7	13.2
	10	11.9	12.0	11.7
	15	10.6	11.4	12.1
	20	10.7	11.4	12.2
	25	10.6	10.5	13.7
Meyer	undef	11.4	11.8	13.9

Table 5.4. Experimentally determined ideal order for each wavelet family.

Wavelet Family	Ideal Order (M^*)		
	Free Air	Leaf	Insect
Daubechies	7	8	8
Coiflet	4	5	4
Symlet	6	7	11

Table 5.3 provides a summary of the results of the tests. The results indicate that the wavelet denoising procedure was very successful in denoising the terahertz pulses, providing an improvement in SNR ranging from 5 dB up to 10 dB. A typical result of the denoising process is shown for the leaf terahertz response in Fig. 5.6. All of the wavelets tested provided similar results however by averaging the results over each wavelet family the families could be ranked in order of decreasing quality to yield: Coiflet, Symlet, Daubechies and Meyer. For each wavelet family the variation of denoised SNR with order was analysed. It was found that for each family there was an ideal order, M^* for which the denoised SNR was maximised. For orders $M < M^*$ the SNR dropped off rapidly and for higher orders $M > M^*$ the denoised SNR dropped off more gradually in a complex fashion approximating an exponential decay overlaid with an oscillatory function. An example of this response is shown in Fig. 5.7 for the Daubechies family. The ideal order for each wavelet was also found and is shown in Table 5.4.

The Wiener Filter

To provide an indication of the power of wavelet denoising for this application it is compared with *Wiener filtering*. The Wiener filter is the classic filter used for noise reduction (Castleman 1996). Given a signal $s(k)$ corrupted by noise $n(k)$, we desire to filter the resulting signal to yield $y(k)$ as close as possible to $s(k)$. If we assume that the signal and noise are stationary, ergodic, random variables of known power spectral densities (PSD), and further that the noise is uncorrelated with the signal, the optimal filter in the sense of mean square error is given by

$$H_o(\omega) = \frac{P_s(\omega)}{P_s(\omega) + P_n(\omega)}, \quad (5.14)$$

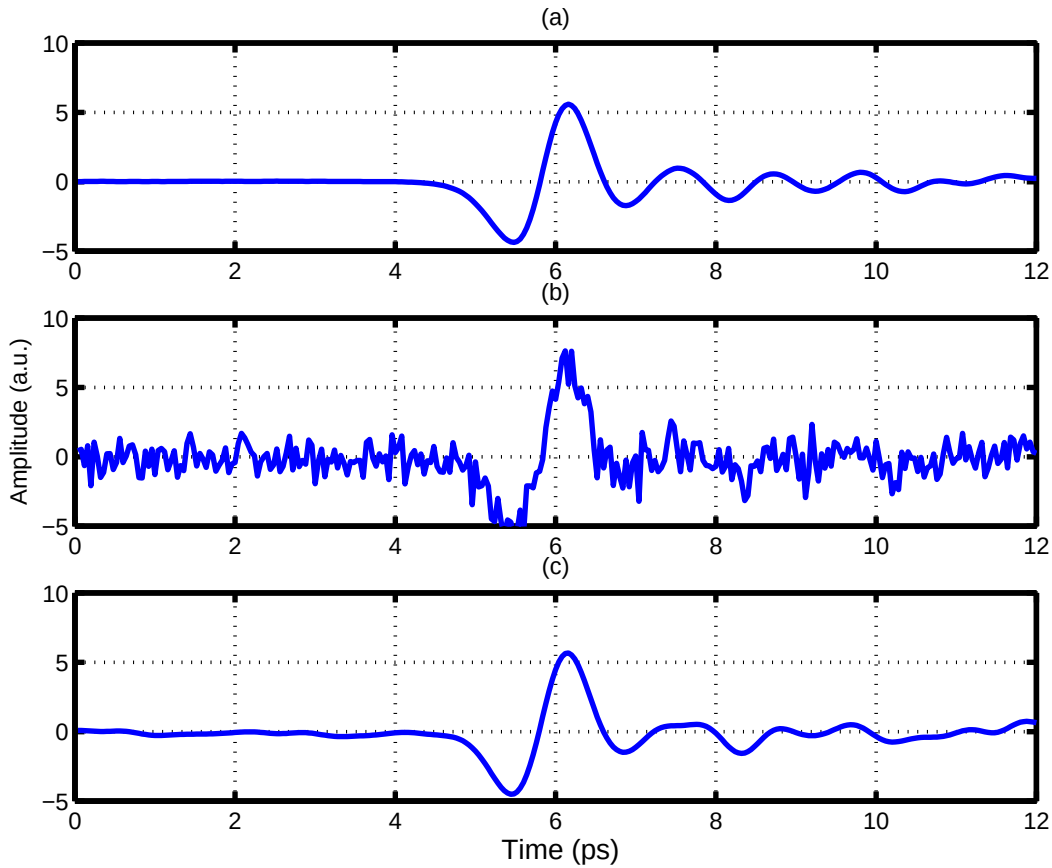


Figure 5.6. Results of wavelet denoising the T-ray response for a leaf. (a) Shows the original response before noise was added, (b) shows the response in (a) with noise added such that the SNR was 3 dB, (c) shows the response in (b) after wavelet denoising was performed using the Coiflet order 4 wavelet. The resultant SNR is 12.1 dB.

where $H_o(\omega)$ is the frequency response of the filter, and $P_s(\omega)$ and $P_n(\omega)$ are the PSDs of the signal and the noise respectively. These are estimated using the direct periodogram method (Kalouptsidis 1997) whereby

$$P_s(\omega) = \frac{1}{N} |X(\omega)|^2, \quad X(\omega) = \sum_{n=0}^{N-1} x(n) e^{-j\omega n}, \quad (5.15)$$

where N is the number of samples and $x(n)$ is the input sequence.

Wiener denoising was applied in the same way as wavelet denoising. White noise was added to the THz signals such that the SNR was 3 dB. Wiener denoising was applied using the known noise power and the resultant SNR was measured. This process was repeated for 100 different realisations of the noise and the resultant SNR averaged. It was found that Wiener denoising is inferior to *all* the wavelet denoising filters tested.

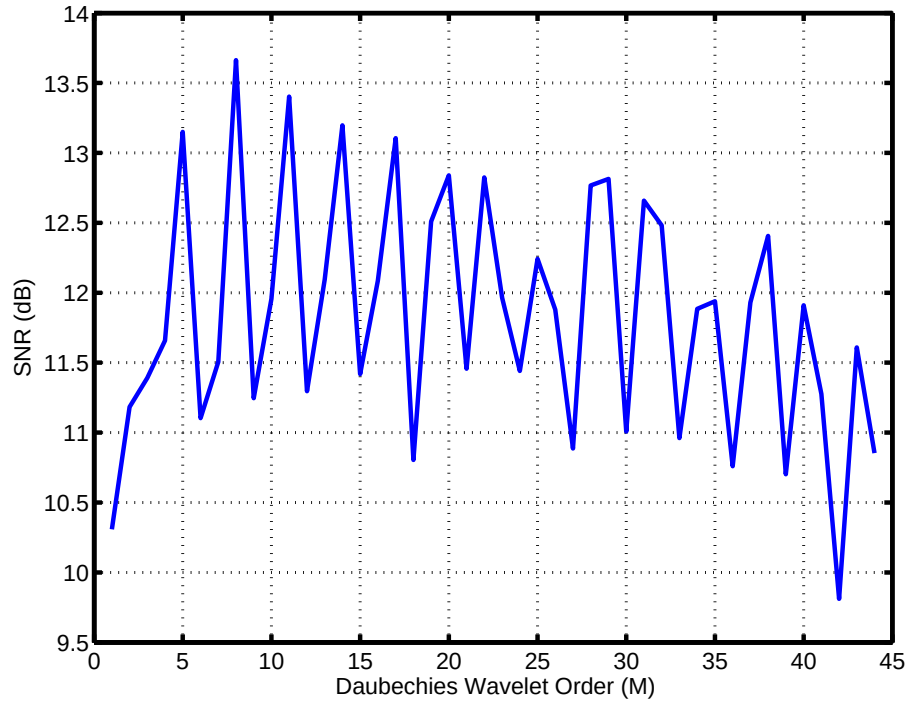


Figure 5.7. Variation in denoised SNR vs wavelet order M . A noisy terahertz pulse (SNR = 3 dB) was denoised with Daubechies wavelets of order M . For each M the resultant SNR was measured and is shown above.

It provided a resultant average SNR of 7.6 dB, 7.3 dB and 7.8 dB for the free air, leaf and insect responses respectively. This highlights the fact that the THz pulses are obviously non-stationary, and that stationary signal processing techniques are therefore inferior to time-frequency methods such as wavelet denoising. Figure 5.8 illustrates the performance of the Wiener denoising filter applied to the noisy leaf response. Comparing this figure to the results of wavelet denoising depicted in Fig. 5.6 clearly reveals the improved capabilities of the latter technique.

5.2.4 Deconvolution

This section considers the problem of estimating the impulse and frequency response of the sample under test from the measured data, as formulated in Sec. 5.2.2.

We have shown in the previous section that frequency domain methods, with their implicit assumption of ergodicity, are often far from optimal for pulsed THz data. However, a wide range of applications of THz-TDS require estimation of the frequency

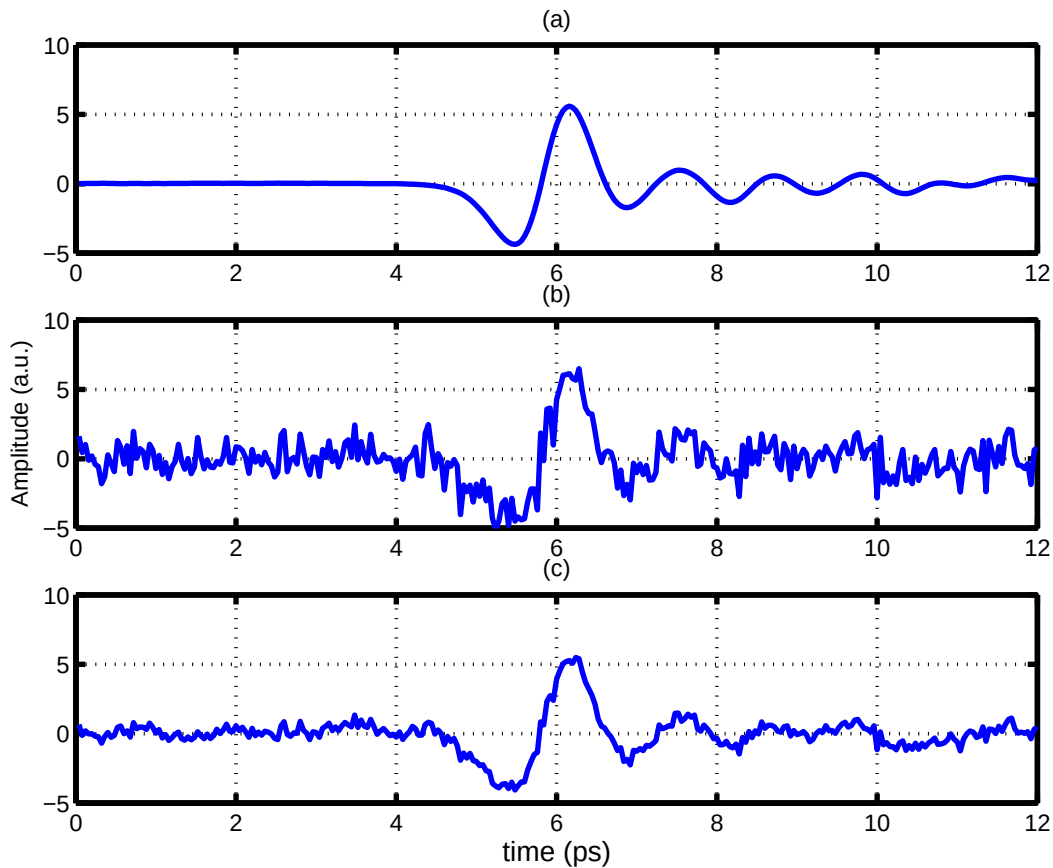


Figure 5.8. Results of Wiener denoising the T-ray response for a leaf. (a) Shows the original response before noise was added, (b) shows the response in (a) with noise added such that the SNR was 3 dB, (c) shows the response in (b) after Wiener denoising. The resultant SNR is 7.4 dB.

response of the sample under test. In these cases the frequency resolution is often critical and it is necessary to process the data in the Fourier domain. In these cases the process of deconvolution is almost invariably applied. It involves dividing the sample spectral response by the system frequency response. Deconvolution was discussed in Sec. 4.6.5 and the problem of phase unwrapping was highlighted. A further problem often encountered in deconvolution of THz data is the implicit amplification of noise at frequencies where there is very little signal power. Deconvolution calculates the ratio of the target and system response in the frequency domain. As THz signals are largely bandlimited, the denominator at frequencies outside this band becomes very small. Any noise present in the signals at these frequencies is then amplified.

One solution to this problem is to follow the deconvolution process with a Wiener filter. It is then referred to as Wiener deconvolution. Figure 5.9 illustrates this process.

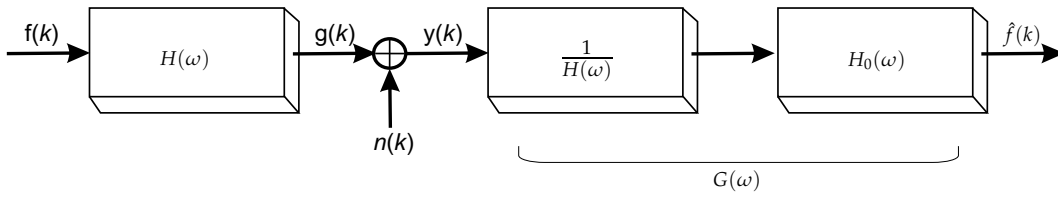


Figure 5.9. Block diagram illustrating the process of Wiener deconvolution. Here, $G(\omega)$ represents the Wiener deconvolution filter. It consists of a deconvolution filter, followed by a Wiener filter. The output $\hat{f}(k)$ is an estimate of $f(k)$. After (Castleman 1996).

The input to the Wiener filter, $H_0(\omega)$ can be seen from Fig. 5.9 to be $f(k) + n(k) * h^{-1}(k)$. Therefore the Wiener filter transfer function is given by

$$\begin{aligned} H_0(\omega) &= \frac{P_f(\omega)}{P_f(\omega) + \frac{P_n(\omega)}{|H(\omega)|^2}}, \\ &= \frac{|H(\omega)|^2 P_f(\omega)}{|H(\omega)|^2 P_f(\omega) + P_n(\omega)}. \end{aligned} \quad (5.16)$$

The transfer function of the deconvolution filter $G(\omega)$ is then given by

$$G(\omega) = \frac{H_0(\omega)}{H(\omega)} = \frac{H^*(\omega) P_s(\omega)}{|H(\omega)|^2 P_s(\omega) + P_n(\omega)}, \quad (5.17)$$

where $H^*(\omega)$ denotes the complex conjugate of $H(\omega)$.

Experimental Deconvolution

The Wiener filter described above was applied to THz data obtained by imaging a 0.6 mm thick slice of Spanish ham ('Jamon Serrano'). The data was obtained using the scanning THz imaging system described in Sec. 3.3.1. Two sections of the ham were considered, one was an area with a high concentration of fat, the other was an area with a low fat concentration, the frequency spectra for these two samples are shown in Fig. 5.10. Wiener deconvolution was applied to each of these samples, for this purpose the Fourier transform of the free air T-ray pulse $x(k)$ was used as $F(\omega)$, the sample T-ray response $y(k)$ was used to determine $P_s(\omega)$ and Gaussian white noise was added to both sequences such that the SNR of each sequence was 3 dB. This was done to illustrate the performance of the filter in the presence of a large amount of noise.

Wiener deconvolution has been illustrated previously for gas responses (Mittleman et al. 1998a), the response of simple gas mixtures to THz radiation is relatively simple

and can be accurately predicted, however the responses shown here are much more complicated as the response of biological tissue results from numerous inter-molecule interactions. The data shown here is representative of the problem encountered when analysing human tissue.

Figure 5.11 shows the results of Wiener deconvolution applied to the ham responses. It can be seen that the fat is relatively transparent to terahertz radiation so the deconvolved response is quite flat (up to 3 THz) whilst the meat has a complex terahertz response, deconvolution therefore makes the task of distinguishing between the two samples easier.

5.2.5 Comparison of Techniques

To conclude this section on THz preprocessing, Fig. 5.12 provides a visual comparison of the preprocessing techniques discussed. Consider the original image shown in Fig. 3.12 with noise added to each response such that the SNR was 3 dB. This is shown in Fig. 5.12(b). The rest of the figure shows the result of wavelet denoising, Wiener deconvolution and the combination of the two techniques on the image quality. The wavelet denoising was performed, using the procedure described in Sec. 5.2.3, using a Coiflet wavelet of order 4. Wiener deconvolution was performed, as described in Sec. 5.2.4, using the average free air pixel response as the system response. In all cases the image was produced by taking the Fourier transform of the processed T-ray pulses and plotting the magnitude of the Fourier coefficient corresponding to a frequency of 1 THz. This is an arbitrary scheme that produces good quality images. It can be seen that wavelet denoising provides a marked improvement in image quality, whilst deconvolution appears to offer little – however deconvolution promises greater benefits for use with classification algorithms, as discussed in subsequent sections.

We also show the results of wavelet denoising applied to the THz responses shown in Fig. 5.2. Moreover, Figure 5.13 shows the results of denoising the signal measured with a small time constant (1 ms) using a Coiflet order 4 wavelet. It can be seen that the noise is significantly reduced, the SNR was improved from 7 dB to 8.5 dB. This technique therefore has the potential to allow effective systems to be constructed without the LIA, this would reduce the hardware complexity and promises to dramatically increase the acquisition speed of the system. To illustrate this point, the algorithms required to generate Fig. 5.12(c) took less than 2 minutes running on a SPARC Ultra 60

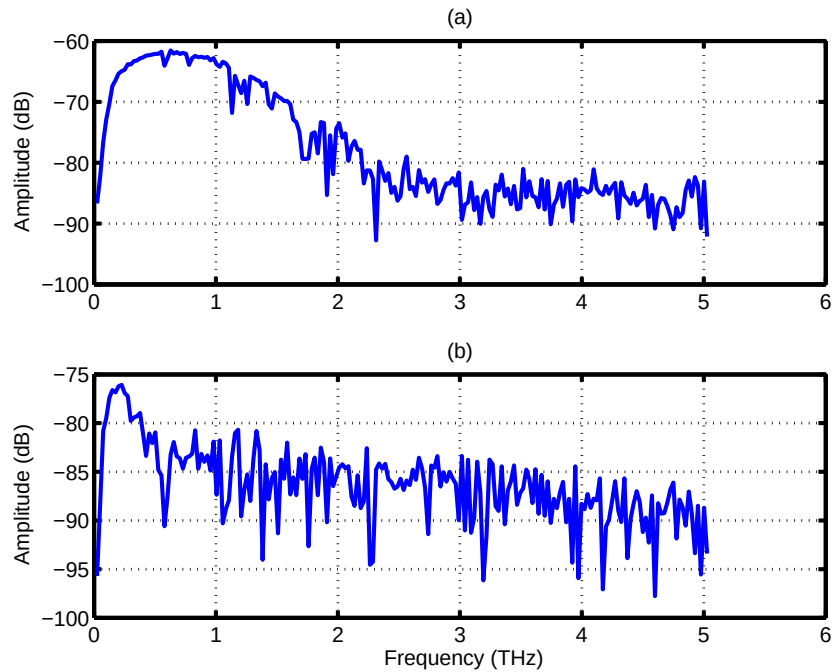


Figure 5.10. Frequency spectrum for two pixels on a piece of Spanish ham ('Jamon Ser-rano'). (a) Shows the spectrum for a pixel corresponding to a high fat region, while (b) shows the spectrum for a pixel corresponding to a lean region.

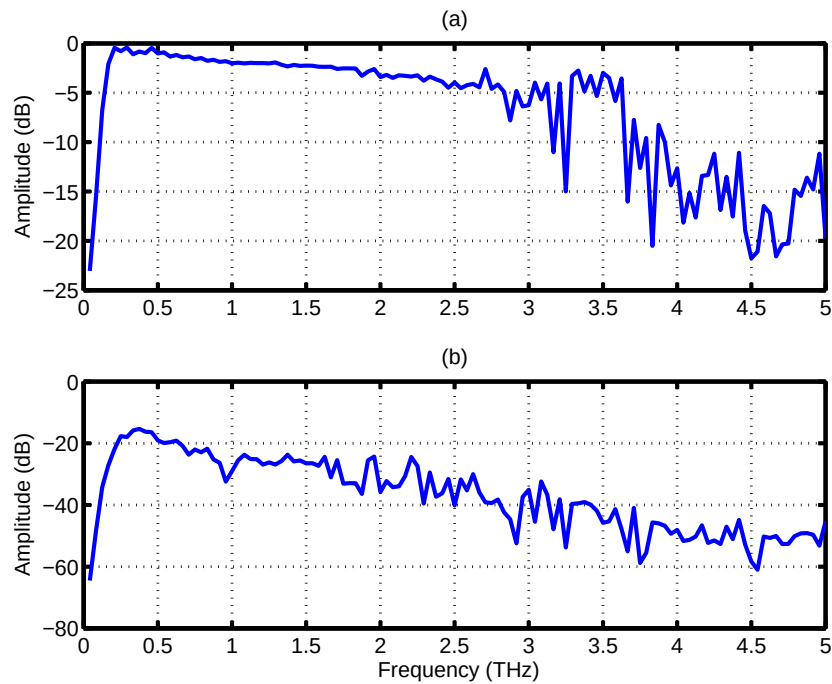


Figure 5.11. Frequency spectrum of ham T-ray pulses after Wiener deconvolution. (a) Shows the deconvolved spectrum for a pixel corresponding to a high fat region, while (b) shows the deconvolved spectrum for a pixel corresponding to a lean region.

5.2 Preprocessing

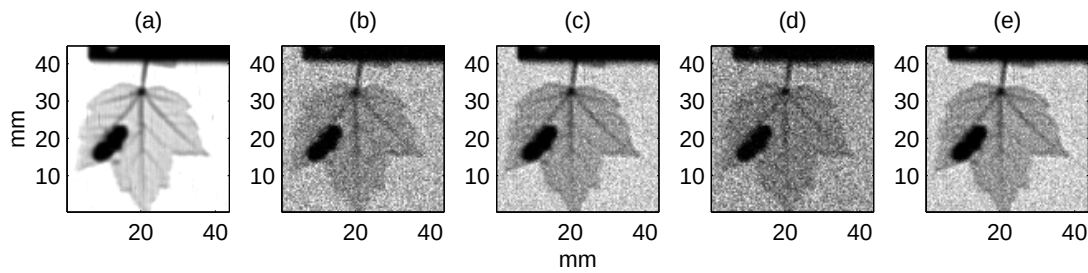


Figure 5.12. A comparison of T-ray images before and after various processing stages. (a) Represents the original noiseless image, (b) shows the same image after noise was added. (c) Shows the noisy image after wavelet denoising using a Coiflet wavelet of order 4, (d) shows the noisy image after Wiener deconvolution, and (e) shows the noisy image after wavelet denoising followed by Wiener deconvolution.

processor at 500 MHz, utilising 512 MBytes of RAM. This is over an order of magnitude faster than the data acquisition process. Wavelet denoising also increases the power of the THz imaging technique in measuring samples that have higher attenuation and correspondingly higher relative noise levels. This is of particular benefit to biomedical applications where the attenuation is typically high.

5.2.6 Conclusion

Soft wavelet denoising was found to be well suited for THz pulse preprocessing, achieving up to 10 dB improvement in SNR when applied to waveforms with initial SNRs of 3 dB. An experimental investigation was performed to determine the ideal wavelet family and order for the denoising application. The results of this experiment are not decisive but a number of useful conclusions may be drawn. Four wavelet families were compared and their performance, although similar, could be ranked in order of success to yield Coiflet, Symlet, Daubechies and Meyer, in order of decreasing average resultant SNR. The order of wavelets within the families were also compared, where the order determines both the number of vanishing moments and the support width of the wavelet. The ideal order for each wavelet family was identified.

This is a dynamic field of research and much work remains. In particular signal processing strategies must be adapted to deal with $1/f$ noise originating from the ultrafast laser, and chirped, single shot terahertz responses (Jiang and Zhang 1998a, Jiang and

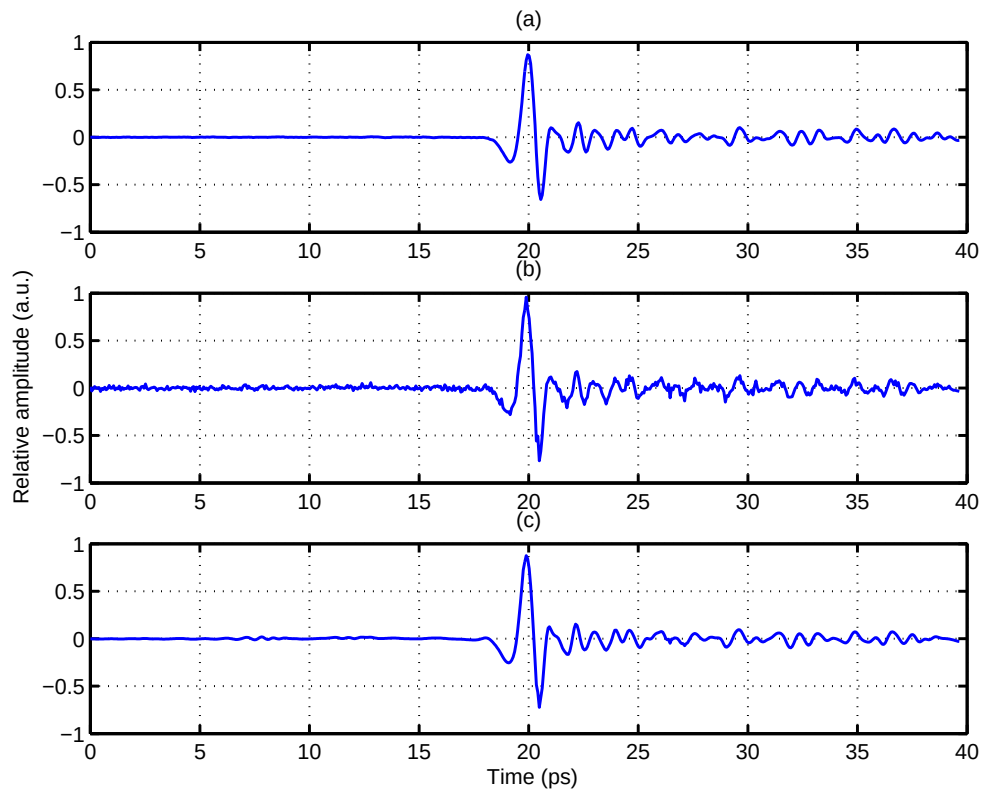


Figure 5.13. Wavelet denoising of THz data measured with a short LIA time constant. (a) Shows a terahertz response measured with a LIA time constant of 100 ms, (b) shows a noisy version of the same signal, measured with a LIA time constant of 1 ms, (c) shows the result of wavelet denoising applied to the signal in (b).

Zhang 1998c). Many other signal processing techniques hold potential; notably adaptive signal processing, and techniques adapted from speech recognition applications.

Future work in this domain will focus on using the wavelet transformed THz data for information processing and classification. Several research groups are active in this area. Galvão et al. (2003) and Handley et al. (2004) have shown that the wavelet transform has promise as a method of feature extraction for material classification. Other applications include THz image data compression (Handley et al. 2002) and THz refractive index estimation (Handley et al. 2001).

5.3 Feature Extraction

In statistical pattern recognition, a pattern is expressed in terms of d features or measurements. Each target is reduced to a point in a d -dimensional space. The goal of feature extraction is to select features such that the samples drawn from each class are clustered together in this d -dimensional space, and the clusters resulting from different classes are well separated.

In this ideal case very simple decision boundaries may be constructed to allow future samples to be accurately classified. Occam's razor is often applied to classification problems. It states that 'Entities (or explanations) should not be multiplied beyond necessity,' (Duda 2001). In the field of pattern recognition this is taken to imply that the simplest classifier that fits the training data should be used. Several studies have shown that simple classifiers do indeed perform well in the majority of circumstances (Holte 1993). And the problem of 'overfitting,' where complex classifiers such as neural networks result in overly detailed decision boundaries that match the training data too closely and thus fail to generalise accurately, is the subject of extensive research (Domingos 1999, Cubanski and Cyganski 1995, Freund 2001).

This makes the question of feature extraction ever more paramount. If a simple classifier is desired, the separation of classes in the feature space is essential. A variety of mathematical transforms such as principle component analysis and linear discriminant analysis (LDA) are commonly used for feature extraction (Jollif 1986, McLachlan 1992). However, these methods are not a universal panacea. Principal component analysis decomposes the data set into a lower dimensional representation that accounts for most of the variance in the data. Unfortunately maximum variance does not always correspond to maximum discrimination between classes (Duda 2001). One disadvantage is the fact that they do not incorporate any domain knowledge of the problem, nor are they able to be used to infer such knowledge.

For these reasons this work has focused on developing feature extraction methods with intuitive justifications in the problem space. This was done in the hope that they, in addition to proving high classification accuracy, may add to our relatively limited knowledge on the interaction between THz radiation and common materials.

5.3.1 The Curse of Dimensionality

In theory, if the probability density functions for each feature for each class are known, then an ideal Bayesian classifier (see Sec. 5.5.1) can be designed and the classification accuracy only improves as additional features are added. However, in practice the probability density functions are seldom known and must be estimated from the training data. In this case, for a given set of training data, as the number of features is increased, the number of free parameters that must be estimated is also increased. This reduces the accuracy of the probability density estimate and the classifier accuracy is correspondingly degraded. This is referred to as the ‘peaking phenomenon’ (Raudys and Pikelis 1980, Trunk 1979) and as the ‘curse of dimensionality,’ which was coined by Richard Bellman in 1961 (Bellman 1961).

Appendix E provides an elegant mathematical demonstration of the Curse of Dimensionality based on (Trunk 1979). The practical result is that classification system design should attempt to select a small number of discriminating features when the training set is of limited size.

5.3.2 System Identification Filter Coefficients

System identification refers to the problem of estimating a system that best describes the measured data. The data is assumed to consist of two sets, $y(k)$ being the output of the unknown system when excited by the input signal $x(k)$. We consider the system S whose output depends on the input signal and on a noise signal $v(k)$

$$\mathbf{y} = S(\mathbf{x}, \nu). \quad (5.18)$$

The identification problem is to determine an estimator

$$\hat{\mathbf{y}} = \hat{S}(\mathbf{y}, \mathbf{x}), \quad (5.19)$$

which minimises some measure of the error signal

$$e(k) = y(k) - \hat{y}(k). \quad (5.20)$$

A common method of solving this problem is to assume that the predictor may be factored using a known transformation $\hat{F}$ and a finite-dimensional parameter θ

$$\hat{S}(\mathbf{y}, \mathbf{x}) = \hat{S}(\mathbf{y}, \mathbf{x}, \theta), \quad (5.21)$$

5.3 Feature Extraction

which is then referred to as parametric system identification. Three common models used in this context are the finite impulse response (FIR) model,

$$\hat{y}(k) = \sum_{i=0}^P c_i x(k-i) + v(k), \quad (5.22)$$

the autoregressive (AR) model,

$$\hat{y}(k) = - \sum_{j=1}^Q a_j y(k-j) + v(k), \quad (5.23)$$

and the ARX model that is a general class combining the two previous examples:

$$\hat{y}(k) = - \sum_{j=1}^Q a_j y(k-j) + \sum_{i=0}^P c_i x(k-i) + v(k), \quad (5.24)$$

where P and Q are the model orders. These models are easily understood as linear filters where the a_j and c_i represent the tap weights (Haykin 1991).

A large number of methods have been proposed to estimate the linear model coefficients (Kalouptsidis and Theodoridis 1993). These methods include iterative gradient descent and the least mean square (LMS) algorithm, which are capable of tracking the optimum coefficients even when the input and output vary with time. These methods form the basis of adaptive system identification.

In this case, it is assumed that the coefficients are constant. The coefficient (or weight) vector $\mathbf{W}$, and the signal vector $\mathbf{U}$ are defined such that

$$\begin{aligned} \mathbf{W} &= [c_0 c_1 \dots c_{P-1} c_P a_1 a_2 \dots a_{Q-1} a_Q]^T, \\ \mathbf{U}_k &= [x(k) x(k-1) \dots x(k-P) y(k-1) y(k-2) \dots y(k-Q)]^T. \end{aligned} \quad (5.25)$$

Equation (5.24) then simplifies to

$$\hat{y}(k) = \mathbf{U}_k^T \mathbf{W} = \mathbf{W}^T \mathbf{U}_k. \quad (5.26)$$

Substituting this expression in Eq. (5.20) yields

$$e(k) = y(k) - \mathbf{U}_k^T \mathbf{W}. \quad (5.27)$$

To minimise the squared error Eq. (5.27) is squared and the expectation is calculated as

$$E[e^2(k)] = E[y^2(k)] + \mathbf{W}^T E[\mathbf{U}_k \mathbf{U}_k^T] \mathbf{W} - 2E[y(k) \mathbf{U}_k^T] \mathbf{W}. \quad (5.28)$$

This equation may be more easily expressed by defining the matrix $\mathbf{R}$ as the ‘input correlation matrix,’ which calculates the expectation of the cross-correlation of the input $x(k)$ and output $y(k)$ data. The expectation is calculated over all time samples $k \in 0..N - 1$,

$$\mathbf{R} = E[\mathbf{u}_k \mathbf{u}_k^T]. \quad (5.29)$$

Similarly defining $\mathbf{P}$ as a column vector

$$\mathbf{P} = E[y(k) \mathbf{u}_k^T]^T, \quad (5.30)$$

allows the mean square error (MSE), η to be expressed as

$$\eta = E[e^2(k)] = E[y^2(k)] + \mathbf{W}^T \mathbf{R} \mathbf{W} - 2\mathbf{P}^T \mathbf{W}. \quad (5.31)$$

This expression is a quadratic function of the weight vector $\mathbf{W}$ and the minimum MSE can be found by differentiating Eq. (5.31) with respect to $\mathbf{W}$ and setting the derivative to zero:

$$\frac{\partial \eta}{\partial \mathbf{W}} = 2\mathbf{R} \mathbf{W} - 2\mathbf{P} = 0. \quad (5.32)$$

Provided $\mathbf{R}$ is nonsingular the optimal weights (filter coefficients) in the mean square error sense are given by

$$\mathbf{W}^* = \mathbf{R}^{-1} \mathbf{P}. \quad (5.33)$$

This equation is referred to as the Wiener-Hopf equation (Wiener 1949, Bode and Shannon 1950, Kailath 1974, Widrow and Stearns 1985). Equation (5.33) may be evaluated using well established pseudo-inverse techniques and fast Levinson’s algorithm methods (Kalouptsidis and Theodoridis 1993).

For analysing the THz data, the THz pulse detected with no sample in place is considered to be the input, $x(k)$, and the THz pulse detected after transmission through the sample is taken as the system output, $y(k)$.

By choosing P and Q as small numbers and evaluating c_i and a_j for a given THz response the time domain pulse is reduced to a small set of features, which are used to allow a classifier to be trained and unknown samples classified. This is demonstrated experimentally in Sec. 5.6.

5.3.3 Deconvolved Frequency Coefficients

THz-TDS is typically used to characterise thin films or planar semiconductor targets. In such cases the THz wave propagation can be easily modeled and the complex refractive index of the material may be extracted using the techniques detailed in Appendix C. In these cases it is natural to use the frequency dependent refractive index as the input to a classification algorithm. For more general targets, with irregular shape and unknown thickness, scattering and diffraction of the THz pulses may significantly distort the time domain signal. This can prevent meaningful extraction of the refractive index.

This section describes a feature extraction method based on the deconvolved frequency dependent transmission function of the target. The deconvolution procedure described in Sec. 5.2.4 is applied to the THz pulses to isolate the material characteristics. However, unlike gas analysis considered in (Mittleman et al. 1998b), most solid materials do not exhibit visibly significant sharp absorption resonances. This is due, in part, to *spectral broadening*. A key reason why absorption spectra are broader in solids than gases is related to the reduced lifetime, τ , over which an atom can be found in its lower absorbing state. This lifetime is reduced in solids due to increased interatomic collisions. This effect is known as *collisional broadening* and the spectral width is given by $\Delta\omega = 1/2\pi\tau$ (Eisberg 1961).

A typical THz-TDS system provides a frequency resolution of 37.5 GHz and a useful bandwidth of approximately 2.5 THz, therefore there are up to $\frac{2500}{37.5} = 67$ usable frequency coefficients. In practice these coefficients will contain much redundant and irrelevant information and a classifier based on all 67 frequency components will prove computationally inefficient and will have poor generalisation performance as a result of the Curse of Dimensionality discussed in Appendix E.

Normalisation

We deconvolve the measured THz responses by dividing the frequency domain responses by the reference THz spectrum that is measured without a sample in place. Due to the coherent properties of THz-TDS this yields the amplitude $A(f)$ and phase $\phi(f)$ of the sample response at each frequency, f , so both of these components are available as potential classification features. One important goal of a THz inspection system is the ability to classify different materials independent of the thickness or amount of the material present. The deconvolved responses are therefore normalised. The

amplitude coefficients are normalised by dividing by the maximum amplitude of the spectrum, while the phase coefficients are normalised by dividing by the phase at the maximum usable frequency (usually approximately 2.5 THz). Mathematically

$$A_{\text{norm}}(f) = \frac{A(f)}{A_{\text{max}}}, \quad (5.34)$$

$$\phi_{\text{norm}}(f) = \frac{\phi(f)}{\phi(f_{\text{max}})}. \quad (5.35)$$

This normalisation procedure is critical to allow a thickness independent classification to be performed as addressed in the case study described in Sec. 5.7.

Fabry-Perot Effects

Another critical aspect of frequency domain classification schemes is the problem of Fabry-Perot effects. These effects are caused by multiple reflections within the target and are a particular problem when considering thin targets with roughly parallel surfaces as discussed in Appendix C. This problem is difficult to combat using post-processing if the geometry and thickness of the target are unknown, however schemes have been proposed to cover several simple cases (Duvillaret et al. 1999, Dorney et al. 2001a).

Fortunately in a majority of cases Fabry-Perot effects can be removed simply by windowing the measured THz pulses. For very thin targets ($< 100 \mu\text{m}$) the target is much thinner than the mean wavelength of the THz pulse and multiple reflections do not arise (Born and Wolf 1999). While for thicker targets multiple reflections will be separated in time by $2(n - 1)l/c$ where l is the thickness of the material, n its refractive index and c the speed of light. A typical THz pulse has a pulse length of 6 ps, so for targets thicker than $900 \mu\text{m}$ with a conservative refractive index of 2, the pulses arising from multiple reflections will be separated in time sufficiently to allow the measured waveform to be windowed to isolate the primary pulse.

Accordingly, an additional step was added to the preprocessing stage whereby the time domain THz pulses are windowed with a 6 ps window around the primary transmitted pulse before deconvolution.

5.4 Feature Selection

How can we compare the performance of different features or feature extraction techniques? This problem is commonly encountered when considering *feature selection*. Typically a large number of features are available and the system designer must choose several from among them to use in the classification system. An obvious technique is to perform an exhaustive search of every possible combination of features and compare their classification accuracy with sample data. However, this technique very quickly becomes computationally prohibitive even for reasonably small numbers of possible features. For example, consider choosing 12 features from among 90 possible options. The total number of combinations is given by ${}^{90}C_{12} = 2.739 \times 10^{14}$! Training and testing a classifier for each of these combinations is clearly impractical. The following sections consider alternative techniques for reducing this computational complexity.

5.4.1 Statistical t-test

A commonly encountered statistical problem is that of determining whether two independently obtained samples are drawn from populations with equal means. To solve this problem it is common to use the Student's⁴ t-test (Phipps and Quine 1995). This test assumes that the two populations a and b are normally distributed with means μ_a and μ_b and the same variance σ^2 . The samples $\{a_i | i = 1, \dots, n_a\}$ and $\{b_i | i = 1, \dots, n_b\}$ are used to estimate the sample means

$$\begin{aligned}\bar{a} &= \frac{1}{n_a} \sum_{i=1}^{n_a} a_i, \quad \text{and} \\ \bar{b} &= \frac{1}{n_b} \sum_{i=1}^{n_b} b_i.\end{aligned}\tag{5.36}$$

⁴'Student' was the pseudonym of the mathematician W. S. Gosset. He was born 13 June, 1876, in Canterbury, England, and died 16 October, 1937, in Beaconsfield, England. He worked as a chemist in the Guinness brewery in Dublin. There, he invented the t-test to statistically handle small samples for quality control in brewing.

And the common variance σ^2 is estimated by the pooled estimate s^2 based on the estimated variance of each sample set

$$s_a^2 = \frac{1}{n_a - 1} \sum_{i=1}^{n_a} (a_i - \bar{a})^2, \quad (5.37)$$

$$s_b^2 = \frac{1}{n_b - 1} \sum_{i=1}^{n_b} (b_i - \bar{b})^2, \quad (5.38)$$

$$s^2 = \frac{(n_a - 1)s_a^2 + (n_b - 1)s_b^2}{n_a + n_b - 2}. \quad (5.39)$$

The test statistic τ is then defined as

$$\tau = \frac{\bar{a} - \bar{b}}{\sqrt{s^2 \left(\frac{1}{n_a} + \frac{1}{n_b} \right)}}. \quad (5.40)$$

It is easy to show that if $\mu_a = \mu_b$ then the numerator of Eq. (5.40) is a normally distributed random variable, however the denominator of Eq. (5.40) is not a constant but is also a random variable. As a result the statistic τ can be shown to have a t distribution with $n_a + n_b - 2$ degrees of freedom (Phipps and Quine 1995).

In the context of feature selection the t-test may be used to evaluate the quality of a feature with regard to the training data. For a given feature, the training data for two classes a and b can be used to estimate the value of τ for this feature. The t tables can then be used to provide the probability that the training data is indeed drawn from two different classes. In this way τ provides a measure of the quality of the chosen feature in differentiating between the two classes. This can be used to provide a very simple method to rank features in order of quality and to allow poor features to be discarded. For the case where there are more than two training classes, similar statistical methods may be used based on *analysis of variance* techniques (Freedman et al. 1991).

The statistical t-test is useful for providing an initial comparison of feature extraction methods and to enable very poor features to be discarded. However it suffers a number of disadvantages when used for feature selection. One disadvantage of this method is that it only allows one feature to be compared at a time, while the ultimate classifier is based on the combination of a number of features. An intuitive method is to simply combine the features that result in the highest individual separation between classes. However, it has long been demonstrated that this is not necessarily optimal and in some cases is spectacularly far from optimal (Cover 1974). A second problem is that maximum separation between training data classes does not necessarily maximise the generalising abilities of a subsequent classifier. Consequently more detailed techniques are required.

5.4.2 Classification Accuracy

A more flexible (and computationally expensive) method of comparing different features is to use the given features to train a classifier with a set of training data and then measure the accuracy of the classifier when applied to a separate set of test data. This method additionally tests the ability of the classifier to generalise based on the information present in the features. Naturally this method is dependent upon the classifier selected as well as the training and test data sets adopted.

Given a set of d possible features, we desire to select a subset of these such that the classification error for the sample data is minimised. The *only* guaranteed method of selecting the optimal subset is to sequentially consider every possible combination of features (Cover and Van Campenhout 1977). This requires that a prohibitively large set of features be considered and is generally not feasible for realistic pattern recognition problems, where typically very large numbers of potential features are available.

A number of iterative feature selection methods have been devised to avoid the necessity of an exhaustive search and while they cannot guarantee optimality they have shown to provide good performance in most practical situations (Jain and Zongker 1997). An example is the Sequential Forward Selection (SFS) algorithm, as described in Jain and Zongker (1997). In this method the single best feature is selected, and features are added one at a time, where the added feature in combination with the previously selected features minimises the classification error. This method is computationally attractive but has the disadvantage that features may never be discarded once selected. Floating search methods, which iteratively add and discard features, overcome this disadvantage at the cost of additional computational complexity (Pudil et al. 1994, Somol et al. 1999).

We adopt an alternative approach to these methods, and use a genetic algorithm to search the feature space and identify optimal feature sets.

5.4.3 Genetic Algorithms

Genetic algorithms are inspired by the theory of biological evolution and follow the principles of mutation and survival of the fittest (Holland 1962, Fogel et al. 1966). Genetic algorithms are an efficient method of iteratively searching a large sample space and arriving at near-optimal solutions based on some *fitness* function. This is achieved

by defining a mathematical representation of each possible solution as a binary string, which is referred to as a *chromosome*. Several potential solutions are created and defined as the initial *population*. The fitness of each member of this population is calculated and the members are ranked according to their fitness score. Only the fittest members are retained for the next generation. Thus simulating the principle of survival of the fittest. The surviving members are then stochastically altered using several evolutionary rules to derive new potential solutions. The fitness of these solutions are calculated and the process repeated until a certain fitness limit is reached or a specified number of generations are tested.

A key advantage of GA's, over other types of stochastic optimisation methods, is their low prerequisites. One simply specifies the variables to be optimised, the environment for evaluation and the genetic operators. No understanding of the underlying input-output model is required by the algorithm.

Genetic Operators

There are three principle operators that take members of a previous generation and derive *offspring*, or child members, for the subsequent generation. These operators, depicted in Fig. 5.14, are replication, crossover (or mating) and mutation:

Replication A chromosome from generation k is simply reproduced, unchanged, in generation $k + 1$,

Crossover Two parent chromosomes are combined (or *mated*) by choosing a split point randomly along the length of the chromosome. The two chromosomes are split at this point and the sections recombined with the matching section from the other parent. This step is one of the keys to the strengths of genetic algorithms as it allows two strong solutions to be combined. The probability that crossover is performed is denoted p_{co} .

Mutation Each bit of a parent chromosome has a small probability p_{mut} of being flipped to derive a mutated child chromosome.

Other operators and variations on these operators abound, however these three form the core of most genetic algorithms (Goldberg 1989, Buckles and Petry 1992).

In the context of the feature selection problem the n potential features are mapped onto an n bit chromosome where each bit (or *gene*) represents a specific feature. If the gene =

5.4 Feature Selection

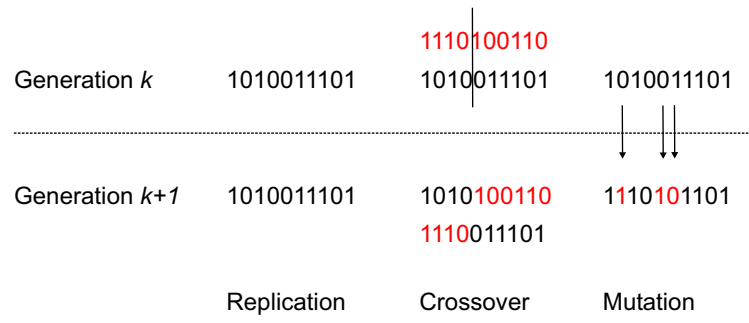


Figure 5.14. Example of the three main genetic operators. These operators govern the chromosomes present in the child generation ($k + 1$) based on those in the parent generation (k). Replication simply copies the parent chromosome. Crossover occurs with probability p_{co} and it splits two parent chromosomes at a random point and joins the matching segments to form two child chromosomes. Finally the mutation operator flips a single bit of the parent chromosome with probability p_{mut} .

1 then that feature is used, otherwise it is not. For example given a frequency resolution of 37.5 GHz the chromosome $[1001010000100 \dots 0]$ indicates that the amplitude and phase coefficients at frequencies of 0.0375 THz, 0.15 THz, 0.225 THz and 0.4125 THz are used by the classifier and all others are discarded.

The fitness function is the classification accuracy using the simple classifier discussed in Sec. 5.5 when trained with a representative set of training data and tested on a separate set of test data. Given these definitions the full genetic algorithm can now be described.

Initially, a population of N chromosomes is randomly selected from the possible combinations. Each chromosome is then assessed by the fitness function to calculate its fitness f_i . The chromosomes are ranked in order of fitness and the maximum fitness is denoted f_{max} . The genetic operators are then applied to the population. Each chromosome is replicated in the next generation with a probability of f_i/f_{max} . Each chromosome is also input to either the crossover or the mutation operator. The probability that the crossover operator is selected is given by p_{co} . Otherwise the mutation operator is selected and each bit has a probability of p_{mut} of being mutated.

The fitness of the new generation of chromosomes is then calculated and the population re-ranked by fitness. A terminating criteria may be defined in terms of an acceptable fitness value or a maximum number of generations. If the terminating criteria is satisfied the algorithm returns the chromosome with the highest fitness. Otherwise any duplicates in the population are removed and the fittest N elements are retained

while the remainder are discarded. The generation is incremented and the genetic operators are again applied to the new generation of chromosomes. This procedure is repeated until the terminating criteria is satisfied. This algorithm is summarised in the flow chart shown in Fig. 5.15. This algorithm was implemented in Matlab using GAOT, i.e. the Genetic Algorithm Optimization Toolbox (Houck et al. 1995).

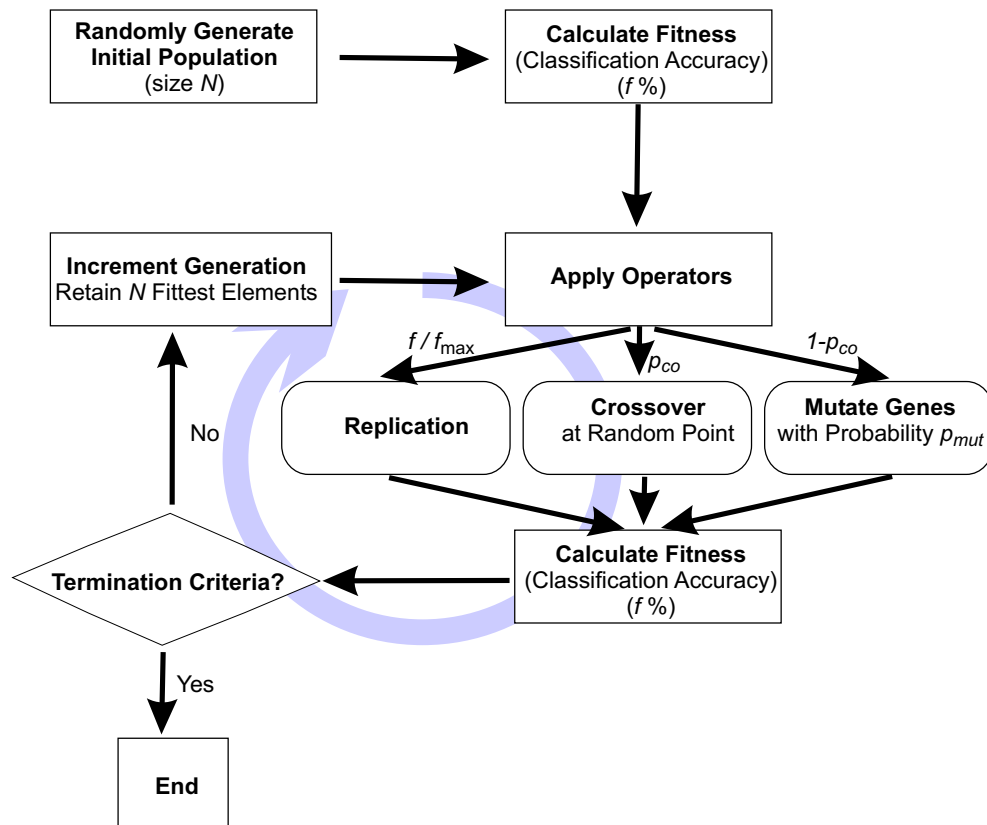


Figure 5.15. Flow chart of a genetic algorithm for feature selection. The algorithm commences by randomly selecting an initial population of size N . The fitness of each element is assessed and the chromosomes ranked according to fitness f . The genetic operators are applied to the population. Each chromosome is replicated with probability $f/f_{\max}$. The chromosomes also pass through either the crossover or mutation operator. The crossover operation takes two parent chromosomes, splits them at a random position and combines the matching sections to produce two child chromosomes, the mutation operator has a low probability of mutating each bit of the chromosome. The fitness of the resulting chromosomes is calculated using the fitness function and the results compared against the terminating criteria, which may be a minimum fitness or a maximum generation. If the criteria is satisfied the highest ranking chromosome is returned otherwise the least fit members of the population are discarded and the process repeats.

Genetic algorithms have been used for feature selection by several authors (Corcoran et al. 1999, Biolot et al. 2003). These authors used the interclass separation of the training data as the fitness function with a penalty term for long feature vectors. The method developed in this Thesis uses the actual classification performance on realistic test data as the fitness criteria. This fitness function measures the ability of the chosen features to allow the classifier to generalise and classify unknown data. It can therefore be expected to result in greater overall classifier performance.

5.5 Classification

It is natural to ask the question: What is the ideal classification algorithm? In the case where the class conditional probabilities are known then the Bayes classifier described in Sec. 5.5.1 provides the solution. However, in practice we rarely, if ever, have access to these probabilities and instead must estimate them from the training data. In this case the question of the optimal classifier is much harder to answer. Say the criteria for judging a classifier is its generalisation performance, or its ability to correctly classify inputs that are not in the training set. It has been shown (Schaffer 1994, Wolpert 1995) that there is *no* context-independent ideal classifier! The *No Free Lunch Theorem* states that for a perfectly general set of test data no one classifier will outperform any other. This is true even if one of the classifiers is notoriously bad, including random guessing or a constant output! This fairly astonishing result implies that the success of one classification algorithm over another in a given context is a result of its suitability to the particular physical properties of the problem including the data distribution, the amount of training data and incorporation of prior information rather than any innate advantages of the algorithm itself.

Consequently the focus of this work departed from the traditionally studied classification algorithms and instead focused on a simple quadratic classifier based on the Mahalanobis distance. This classifier defines simple quadratic decision boundaries in the feature space and relies on the feature extraction method to accurately separate the classes. In this way the classification accuracy is a direct measure of the performance of the feature extraction methods (discussed in Sec. 5.3). In this section we briefly review Bayesian classification to provide a theoretical foundation and then describe the mechanics of the Mahalanobis classifier that was adopted.

5.5.1 Bayesian Classification

“Bayesian decision theory is a fundamental statistical approach to the problem of pattern classification.”

Duda (2001)

Bayesian decision theory is based around the *class-conditional probability density function* $p(x|\omega)$. The feature variable (or vector) x is taken to be a continuous random variable, and there are assumed to be a number of possible classes or states $\omega_1, \omega_2, \dots$. The class-conditional probability density $p(x|\omega)$ is the probability density function for x given that the state is ω . Bayesian decision theory relies on knowing, or estimating, the probability density functions for each possible class. The *a priori* probability of each potential class is denoted $P(\omega_i)$ and is also assumed to be known. Bayes formula is given by

$$P(\omega_i|x) = \frac{p(x|\omega_i)P(\omega_i)}{p(x)}, \quad (5.41)$$

where $P(\omega_i|x)$ is the *a posteriori* probability, the probability that the target belongs to class i given that the feature vector x has been measured. The probability that the feature value x is measured is denoted $p(x)$ and given by

$$p(x) = \sum_{i=1}^N p(x|\omega_i)P(\omega_i), \quad (5.42)$$

where N is the number of potential classes.

An obvious classification scheme is then to minimise the probability of classification error by choosing the class for which the *a posteriori* probability is maximised. Bayes decision rule is then to measure x , calculate $P(\omega_i|x) \forall i \in 1 \dots N$ and select the class ω_i for which $P(\omega_i|x)$ is greatest.

The Bayesian classifier results in the maximum theoretical classification accuracy, however it requires exact and complete knowledge of the class-conditional probability densities – this information is very seldom available. Accordingly a large number of alternate classification methods have been developed. Most of these methods make implicit or explicit assumptions about the form of the class-conditional probability densities and the accuracy of these assumptions is a significant determinant in the accuracy of the classifier.

5.5.2 Mahalanobis Distance

One of the most common and versatile classifiers is the *Mahalanobis distance* classifier (Schürmann 1996). It is one of a class of minimum distance classifiers. It assumes that the data for each class are normally distributed, thus the samples, $\mathbf{x}_i$ drawn from each class will form a cluster in k dimensions, with a centre given by the mean vector, μ , and shape dependent on the covariance matrix, Σ . Estimates are formed for these parameters for each class i , using the training vectors,

$$\mu_i = E[\mathbf{x}_i], \quad (5.43)$$

$$\Sigma_i = E[(\mathbf{x}_i - \mu_i)(\mathbf{x}_i - \mu_i)^T]. \quad (5.44)$$

The *Mahalanobis distance* calculates the distance of a given point from the mean value for a given class normalised by the variance of the training vectors in that direction. For a given class, i , the distance is defined as,

$$d_i(\mathbf{x}) = \sqrt{(\mathbf{x} - \mu_i)^T \Sigma_i^{-1} (\mathbf{x} - \mu_i)}. \quad (5.45)$$

Classification is then performed by selecting the class for which the *Mahalanobis distance* is minimised. This classifier is optimal for normally distributed classes with equal covariance matrices and equal *a priori* probabilities. The covariance matrices were computed for the THz data in the first case study and showed that these assumptions are approximately valid as discussed in Sec. 5.6.3.

In the above discussion we have tacitly assumed that the cost of each decision is equal. In practice this is often far from true. In the third case study described in Sec. 5.8 misclassifying cancerous cells as healthy is likely to be far more costly than the inverse. In this case a cost function would be incorporated into the classifier to bias it towards less expensive errors. A false negative would be penalised more heavily than a false positive. However, this cost function is necessarily application-dependent, and thus we abstract over this detail and for the remainder of this Thesis assume equal *a priori* probabilities and symmetric cost functions.

The Mahalanobis-based classification scheme was chosen because it is simple to implement and it provides reasonable results for a variety of statistical properties, thereby highlighting the performance of the feature extraction techniques. More complicated classification algorithms abound and the appropriate choice for THz applications is an open research area.

5.5.3 Other Methods

Artificial Neural Networks (ANN) are among the most popular classification architectures in use (Haykin 1994). They derive their inspiration from the operation of human and animal brains, which are based on a network of very simple building blocks called neurons. In a similar manner ANNs consist of a network of simple processing elements that conventionally consist of a non-linear activation function applied to the sum of the weighted inputs. The weights of the neurons are adapted to the training data to train the neural network and then the classifier can be used to classify subsequent test vectors.

Support Vector Machines (SVMs) provide another relatively recent approach to pattern recognition that have attracted a great deal of interest for a number of machine learning applications. SVM theory was first introduced by Vapnik (1995) and is based on the principle of *structural risk minimisation*. Intuitively, given the set of samples belonging to two classes, SVMs learn the boundary between these two classes by mapping the input samples to a high dimensional space and then finding a hyperplane in this high dimensional space that separates the samples of the two classes. Computing the best hyperplane is posed as a constrained optimisation problem and solved using quadratic programming techniques.

While these methods have promise in a THz classification setting, they were not pursued in this Thesis as they involve significant design complexity. For example, choosing a neural network architecture and training algorithms are significant research fields in their own right, and others are actively pursuing this work for THz spectroscopy applications (Oliveira et al. 2003). This complexity could obscure the main question under discussion, that of identifying suitable feature extraction techniques to process the THz spectroscopic data. In this context a simple, robust classifier is preferred and hence the Mahalanobis distance classifier was utilised.

5.6 Case Study #1: Tissue Identification

Sections 5.2 to 5.5 have presented a complete THz classification framework including preprocessing algorithms, feature extraction techniques and the Mahalanobis classifier. Armed with this toolset the remainder of this Chapter considers three case studies. These studies served both to test the performance of the preprocessing and classification methods with realistic data, and to demonstrate the applicability of pulsed THz

5.6 Case Study #1: Tissue Identification

imaging systems to several real-world problems. The case studies cover a range of applications from biomedical imaging through to mail inspection. In this first study *ex-vivo* tissue samples of chicken and beef were imaged and THz spectroscopy was used to differentiate between the different tissue types. Several recent studies have considered the characterisation of tissue using THz-TDS (Han et al. 2000a, Walker et al. 2003, Berry et al. 2003). Berry et al. (2003) generated a catalog of the properties of human tooth enamel, cortical bone, skin, adipose tissue and striated muscle. Due to the high absorption of water-rich tissue most work has focused on reflection-mode studies. This case study uses a transmission-mode THz imaging system and dried tissue samples to reduce THz absorption. The goal was not to obtain quantitative tissue properties but to qualitatively demonstrate differentiation between tissues.

5.6.1 Data Acquisition

A number of animal tissue samples were imaged. A beef sample was cut from a beef loin T-bone steak, parallel to the normal steak cut with a thickness of 1.5 mm. To reduce THz absorption due to moisture the sample was pressed and then dried in an oven for 12 hours at 35°C. The sample was held in a sample holder consisting of two 600 μm thick, high density polyethylene sheets and imaged using the chirped probe beam THz imaging system described in Sec. 3.3.3. Polyethylene has negligible absorption in the THz band of interest and only marginal Fresnel loss due to its low refractive index of 1.5. An optical image of the beef sample is shown in Fig. 5.16. The target was imaged using a spatial step size of 1 mm and the THz pulse was measured at each pixel using the chirped probe technique. The THz data was processed to generate the images shown in Fig. 5.17. As illustrated in Sec. 3.3.3 the THz data contains a wealth of information that enables several images to be derived. Three examples are shown in Fig. 5.17(a), (b) and (c). These three images are then combined on different colour axes to form a colour image, shown in Fig. 5.17(d).

Samples of chicken tissue and chicken bone were obtained and imaged in a similar manner. Figures 5.18 and 5.19 show typical time domain and frequency domain THz responses for the beef and chicken samples. The spectral bandwidth of the chirped probe measurement technique and the high absorption of water at high frequency combine to severely limit the bandwidth of the THz measurement as highlighted in Fig. 5.19. Using normal time scanned THz detection the THz bandwidth extends to 1.2 THz for the sample holder response using the same photoconductive antenna THz



Figure 5.16. Optical image of a section of dried beef. The beef sample was cut from a T-bone steak with a thickness of 1.5 mm. The sample was then pressed and dried in an oven at 35°C for 12 hours to remove moisture before THz imaging. After drying the tissue thickness varied between 0.5 and 1 mm.

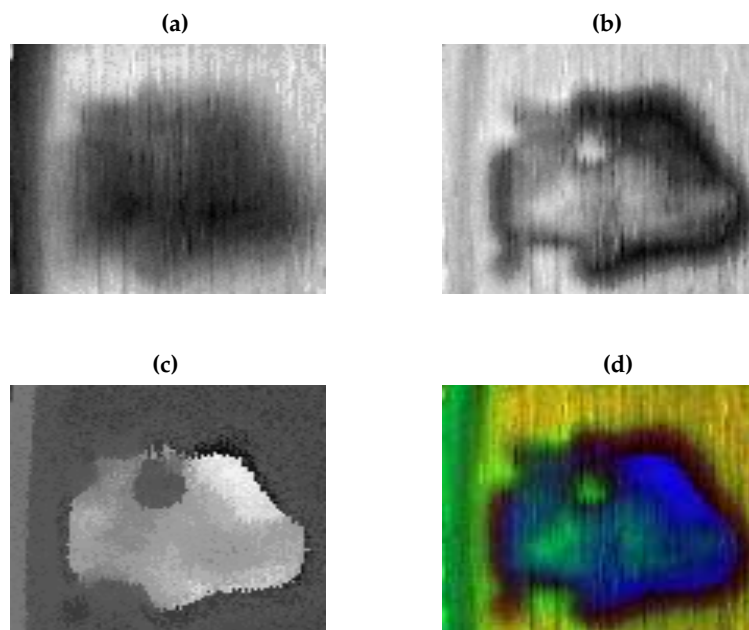


Figure 5.17. Chirped pulse THz images of dried beef. The target was imaged using a spatial step size of 1 mm. The THz pulses at each pixel were processed and used to generate images. (a) Shows the amplitude of the THz pulse at each pixel for a fixed timing sample of 37.5 ps. (b) Shows the peak amplitude of the THz pulses at each pixel. (c) Shows the timing of the peak of the THz pulse, and (d) shows the combination of these three methods with each applied to a different colour axis.

5.6 Case Study #1: Tissue Identification

emitter. This bandwidth limitation severely limits the efficacy of the frequency domain feature extraction techniques described in Sec. 5.3.3 and accordingly this study focused on the alternative technique based on linear modelling for system identification.

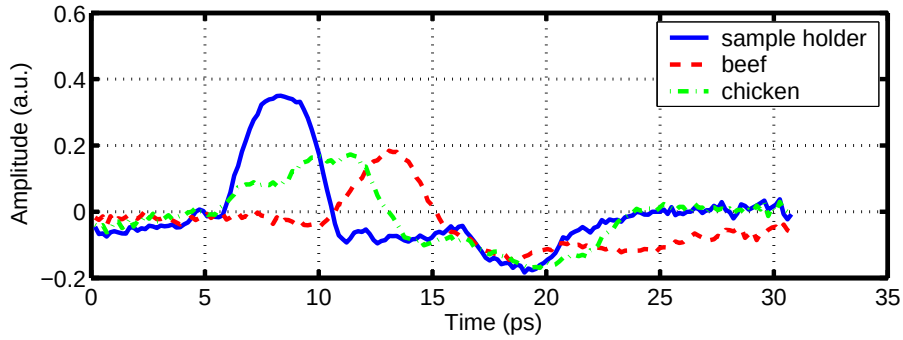


Figure 5.18. THz responses after transmission through beef and chicken samples. The THz responses were measured using the chirped probe beam technique. Thin dried slices of beef loin and chicken breast were placed in a polyethylene sample holder for imaging. The response of the empty sample holder is also shown.

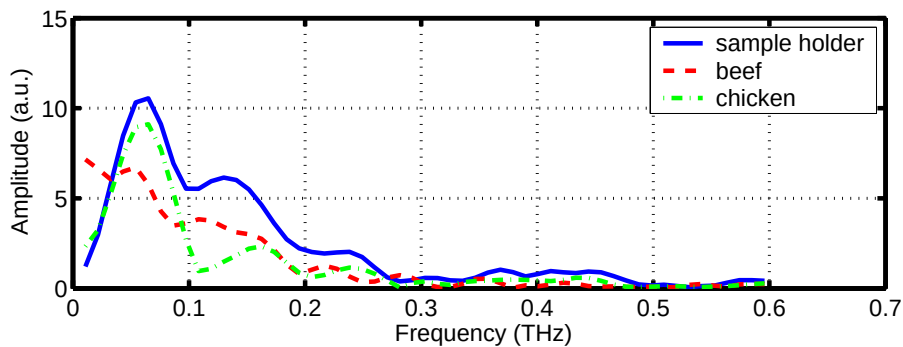


Figure 5.19. THz spectra of the responses shown in Fig. 5.18. The high frequency spectrum is severely limited by high absorption of the tissues and by the limitations of the chirped probe measurement technique.

5.6.2 Linear Modelling

The linear filter models discussed in Sec. 5.3.2 were employed for two reasons, firstly to attempt to infer information about the physical properties of the samples and secondly because the coefficients for an accurate model provide an efficient feature extraction method for the classification problem considered in Sec. 5.6.3.

An ensemble of 50 random pixel responses for each of the chicken and beef samples were chosen. The signals were denoised using the wavelet denoising procedure described in Sec. 5.2.3. The model coefficients for various order AR and FIR models were then computed for each response. For each model the average coefficients were calculated and these were used to calculate the percentage of the average actual response predicted by the model. These results are summarised in Table 5.5. It can be seen that the FIR filter performs much better than an AR filter of the same order. This is in contrast to THz gas spectroscopy results, which are well fitted using AR models (Mittleman et al. 1998a). Gases have very low refractive indices, but show sharp absorption resonances at THz frequencies. These characteristics are well modeled using AR filters. The tissue responses considered here show strong broad frequency-domain features for both absorption and refractive index. These characteristics are more suited to FIR filter modeling. The FIR filter performs competitively with the more general ARX filter model for the same number of coefficients.

The model accuracy η was calculated by the following formula

$$\eta = \left(1 - \frac{\sum_{k=0}^{N-1} |\hat{y}(k) - y(k)|}{\sum_{k=0}^{N-1} |y(k)|} \right) \times 100(\%). \quad (5.46)$$

Figure 5.20 shows an example of the second order FIR and AR filter models with the actual chicken response. It can be seen that the model quite accurately represents the response of the sample. Table 5.5 shows the prediction accuracy of FIR, AR and ARX models for modeling the THz response after transmission through the chicken breast. The prediction accuracy is over 50% for all FIR models with order greater than 2. This is a reasonably good result, considering the amount of noise present in the data.

5.6.3 Classification

The problem considered was that of taking a random THz response and classifying it into one of three different classes: chicken, beef or empty sample holder. Training vectors were chosen at random from among the available responses.

Several different feature extraction methods were tested. It was found that the model coefficients for the FIR model proved to be very reliable features. The Mahalanobis classifier described in Sec. 5.5 was trained using 50 pixel responses for each of the three classes. This resulted in a training set size of 150 samples. To test the classifier 300 random test responses were chosen, and the classifier was used to assign them each

5.6 Case Study #1: Tissue Identification

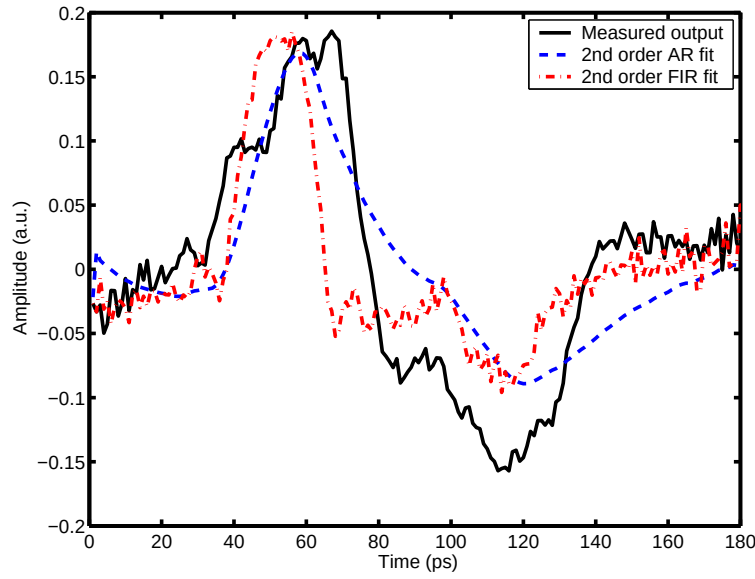


Figure 5.20. Model output for second order FIR and AR filters. The sample holder THz response was used as the model input and the measured response after transmission through the chicken breast was used as the desired output. The least squares model coefficients were calculated using the Wiener-Hopf equation for second order FIR and AR systems. The model outputs are compared with the desired output. The models are modestly accurate, accounting for 43% and 32% of the actual response respectively.

to one of the classes. The training pixels were omitted from the possible test pixels to ensure that the classifier was tested using an independent data set. It was found that using the second order FIR coefficients as features resulted in successful classification of $297/300 = 99\%$ while using the second order AR coefficients gave an accuracy of $289/300 = 96\%$. An intuitively obvious feature extraction method involves simply using the amplitude of the THz pulse and the time at which the maximum amplitude occurred as features. These features give an indication of both the absorption and the phase induced by the sample under test. This intuitive method was tested using the THz data and was found to accurately classify only 283 of the 300 test vectors. The *confusion matrices* for these three respective classifiers are given in Eq. (5.47), where the element, $[i, j]$, shows the relative proportion of samples belonging to class i that were recognised as class j . The classes were free air(1), beef(2) and chicken(3) pixels.

$$\mathbf{X}_{\text{FIR}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.98 & 0.02 \\ 0 & 0.01 & 0.99 \end{bmatrix} \quad \mathbf{X}_{\text{AR}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.92 & 0.08 \\ 0 & 0.03 & 0.97 \end{bmatrix} \quad \mathbf{X}_{\text{amp}} = \begin{bmatrix} 0.99 & 0.01 & 0 \\ 0 & 0.89 & 0.11 \\ 0 & 0.05 & 0.95 \end{bmatrix}. \quad (5.47)$$

Table 5.5. Prediction accuracy for different models. Different order AR, FIR and ARX linear filter models were used to fit a measured THz pulse after transmission through a sample of chicken breast. A free air THz response was used as the system input. The least squares model coefficients were calculated and the model system output generated. The model output was compared with the expected output and the error calculated according to Eq. (5.46).

Model	Order	Prediction Accuracy (%)
AR	2	30.0
AR	3	32.3
AR	4	35.5
AR	5	39.1
AR	6	42.9
FIR	2	43.4
FIR	3	51.0
FIR	4	53.1
FIR	5	56.5
FIR	6	59.4
ARX	2,2	44.8
ARX	3,3	59.8
ARX	4,4	64.6

Figures 5.21 and 5.22 demonstrate the benefits of the FIR model based approach by plotting the distribution of the extracted features for a random set of beef and chicken pixels. The separation of the classes using the FIR model feature extraction method is visibly superior to the intuitive method of using the THz pulse peak amplitude and the timing of the peak.

Covariance Matrices

The Mahalanobis distance classifier reduces to the optimal Bayesian classifier if the following conditions are satisfied:

1. The training data sets are large enough (and representative enough) that the mean and covariance for each class may be estimated accurately.
2. The feature variables are normal random variables, that is, the values of the feature for a given class follow a normal (Gaussian) distribution.

5.6 Case Study #1: Tissue Identification

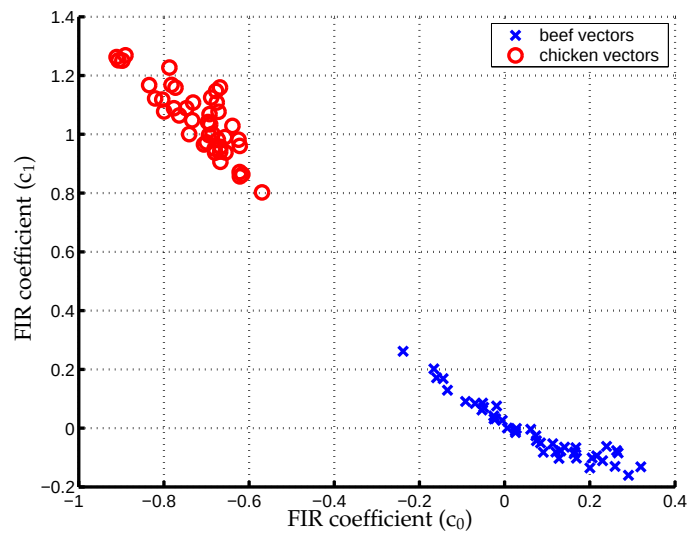


Figure 5.21. Scatter plot showing the discriminating power of the 2nd order FIR model coefficients. The optimal FIR model coefficients are found for 100 random samples and plotted. The two classes show a significant difference in their coefficients.

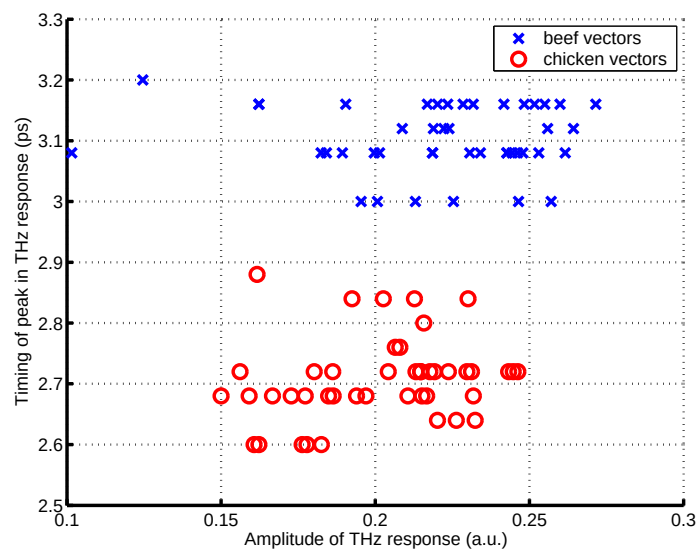


Figure 5.22. Scatter plot showing the distribution of the peak amplitude and the timing of the peak of the THz pulses for beef and chicken samples. There is an obvious difference between the two tissue types but the separation of classes is not as strong as that shown in Fig. 5.21.

3. The covariance matrices for the feature vectors for each class are equal.
4. The *a priori* probabilities for each class are equal.

Conditions 1 and 4 are simply related to the experiment design and are assumed to be satisfied in this case. To verify conditions 2 and 3 the distribution and covariance of the FIR filter coefficients were calculated for the training data. Figure 5.23 shows the histograms for the second order FIR filter coefficients for the beef training data. These distributions show that the amount of training data is sufficient to allow accurate statistics to be estimated and that each variable is approximately normally distributed. A Gaussian fit of the data yielded the curve shown in Fig. 5.23 and the RMS error in the fit was 2.2 for coefficient c_0 and 2.9 for coefficient c_1 . Comparable histograms for the intuitive amplitude and timing features are shown in Fig. 5.24. The RMS error in the Gaussian fit for the amplitude of the THz pulses was 2.8 while for the timing of the THz pulse it was 6.6 indicating that the Gaussian distribution assumption is less valid for these features.

The covariance matrices may be calculated based on the training data for each of the two feature extraction techniques. The covariance matrix is the symmetric, positive semidefinite matrix defined by the elements

$$\sigma_{ij} = E [(x_i - \mu_i)(x_j - \mu_j)] . \quad (5.48)$$

For the second order FIR model coefficients the covariance matrices for the beef and chicken classes are given by

$$\Sigma_{\text{FIR}(\text{chicken})} = \begin{bmatrix} 0.02 & -0.014 \\ -0.014 & 0.011 \end{bmatrix}, \quad \Sigma_{\text{FIR}(\text{beef})} = \begin{bmatrix} 0.016 & -0.009 \\ -0.009 & 0.013 \end{bmatrix}, \quad (5.49)$$

respectively, which are approximately equal. While for the amplitude and timing features the covariance matrices are far from equal:

$$\Sigma_{\text{amp}(\text{chicken})} = \begin{bmatrix} 0.0013 & -0.0002 \\ -0.0002 & 0.0024 \end{bmatrix}, \quad \Sigma_{\text{amp}(\text{beef})} = \begin{bmatrix} 0.0007 & 0.0004 \\ 0.0004 & 0.0052 \end{bmatrix}. \quad (5.50)$$

The FIR coefficients are therefore near optimal features for this problem when combined with the Mahalanobis classifier, as the classifier approaches an ideal Bayesian classifier.

5.6 Case Study #1: Tissue Identification

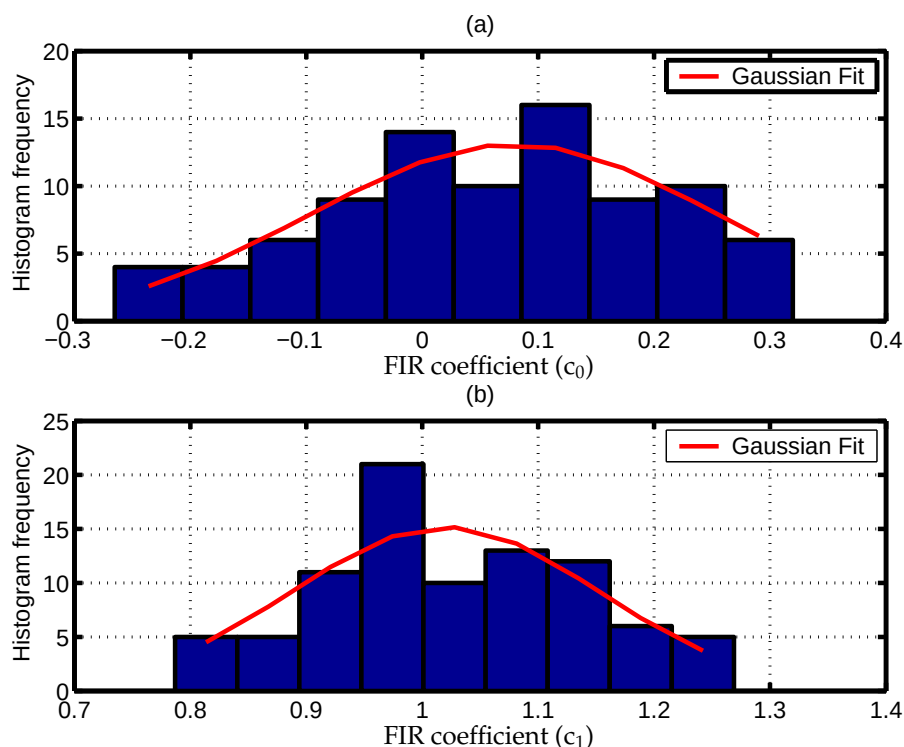


Figure 5.23. Histogram of the 2nd order FIR model coefficients for the beef data. The coefficient values are binned into 10 equally spaced bins and the number of elements in each bin is plotted. For normally distributed variables the histogram should follow a Gaussian curve. (a) Histogram for the first FIR coefficient c_0 . (b) Histogram for the second FIR coefficient c_1 .

Image Classification Example

The following example further illustrates the ability of the chirped probe pulse THz imaging technique to distinguish between biological tissues. It also highlights the ability of the developed classification framework to assist in information extraction. A slice of chicken leg was cut so as to include a section of the bone. The sample was approximately 1.5 mm thick. The sample was then prepared and imaged as described in Sec. 5.6.1. After drying the sample thickness ranged between 0.5 and 1.5 mm. An optical image of the sample is shown in Fig. 5.25. The terahertz data was analysed and it was found that the chicken and bone had a comparable absorption for THz signals and were not clearly distinguishable using standard intensity images. This is illustrated in Fig. 5.26(a), which shows the amplitude image of the chicken sample. Several feature extraction methods were tested and the 5th order FIR coefficients were found to maximise the classification performance. The classifier was trained using 50 reference pixels for each class (bone, tissue and empty holder). The reference pixels were

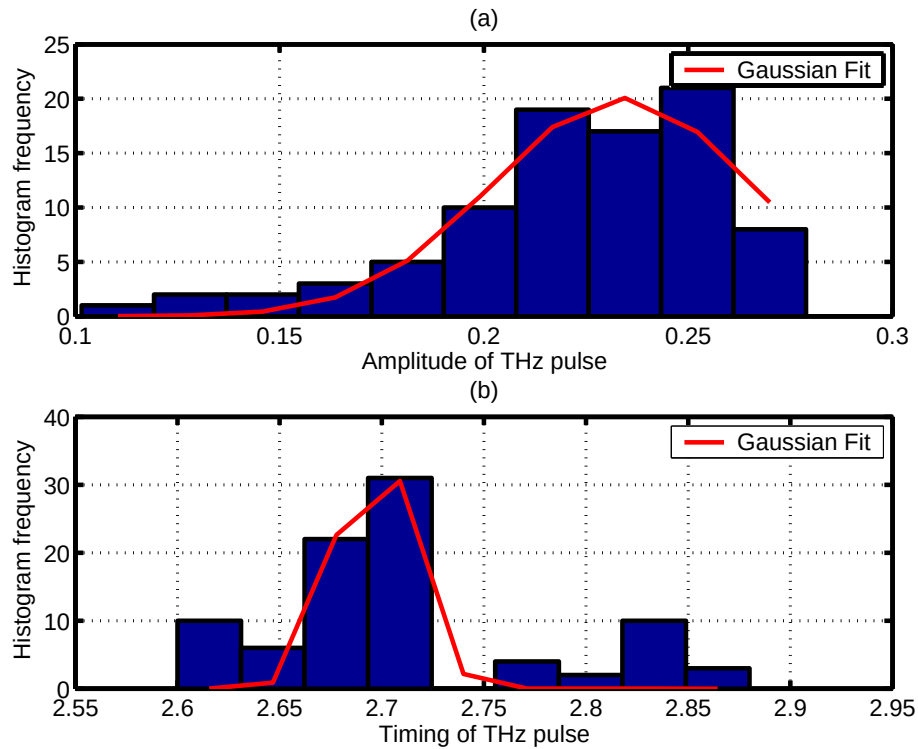


Figure 5.24. Histogram of the peak amplitude and the timing of the peak of the THz pulses.

The beef training data was used to calculate the features. The data was then binned into 10 equally spaced bins and the number of elements in each bin is plotted. It is obvious that this data is not normally distributed. (a) Histogram for the amplitude of the THz pulses, (b) histogram for the timing of the peak of the THz pulses.

chosen based on the geometry of the sample. The classifier was then used to classify all 10,000 pixels of the image into one of the three classes. This classification was then used to colour code the image shown in Fig. 5.26(b). The bone area (green) can be seen to accurately correspond to the bone in the optical image.

5.6.4 Conclusion

We have presented the first ever images of biological tissue measured using the chirped probe pulse THz imaging technique, and have demonstrated the richness of the information content of the obtained data. The developed classification framework allowed automated analysis of these images with high accuracy. Beef and chicken samples were classified using a Mahalanobis distance classifier. The required computational complexity of the classifier was reduced using linear filter models to extract features

5.6 Case Study #1: Tissue Identification

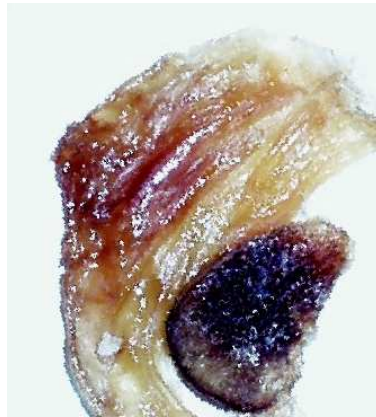


Figure 5.25. A standard optical image of a sample of dried chicken tissue. The bone is clearly visible in the lower right of the image.

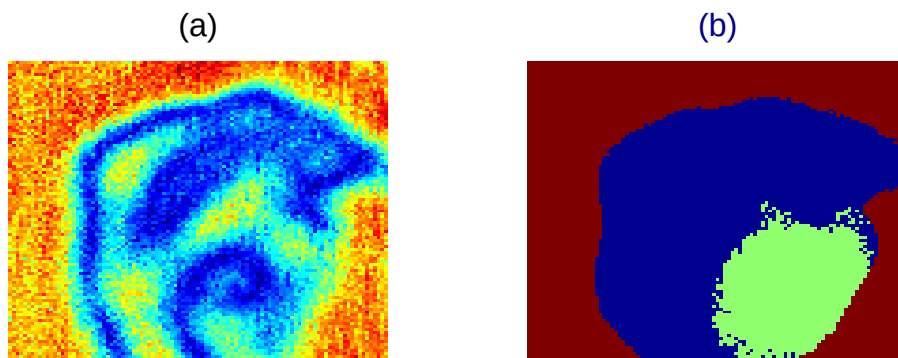


Figure 5.26. Terahertz images of the chicken tissue shown in Fig. 5.25. (a) Shows a THz image generated by mapping the maximum amplitude of the THz pulse at each pixel to the pseudo-colour intensity. Red corresponds to maximum amplitude, violet to minimum amplitude. (b) Shows a pseudo-colour image generated by classifying each pixel of the image based on a number of training pixels that were chosen using knowledge of the original sample geometry. The 5th order FIR filter coefficients were used with a Mahalanobis distance classifier. The pixels classified as free air are shown maroon, chicken tissue pixels show as blue, and bone pixels are shaded green.

from the measured responses. Different filter models were compared and very simple second order FIR filters were found to perform surprisingly well indicating that this model may be an accurate approximation of the underlying physical system. Further investigation of a physical model for the interaction of THz radiation with tissue is an important open question and it is likely to yield vastly improved feature extraction and classification algorithms.

The computational complexity of the algorithms are a vital concern as systems head towards real-time data acquisition. The total time taken to classify the 10,000 responses in Fig. 5.26 was less than 11 seconds on a Pentium IV PC with 256 MBytes of RAM. This is an over an order of magnitude less than the acquisition time for the same image and could be improved further by optimising the software implementation.

5.7 Case Study #2: Powder Detection

The detection of potentially hazardous materials inside mail and luggage has become a top worldwide priority in recent years. Bacterial spores such as *Bacillus anthracis* have been of particular concern since they were used in suspected mail bioterrorism attacks leading to 5 deaths in 2001 (Douglass 2003). Figure 5.27 shows one of the letters used in the 2001 terror attacks and is reproduced from an FBI press release. Several technologies are under development and on the market for detecting hazardous material in mail, however the search continues for a real-time, highly sensitive, highly specific, yet general purpose imaging detection system.

Recent experiments on bacterial spores including the anthrax simulant *Bacillus subtilus* have demonstrated several strong attenuation resonances in the THz frequency range (Globus et al. 2002). These resonances are attributed to the protein cladding of the spore (Brown et al. 2002). These results promote the possibility of allowing automatic detection or *retection*⁵ of bacterial spores concealed within mail. However, detection of powdered materials presents additional difficulties compared to the previously published thin film studies. Most powders strongly scatter THz radiation. The scattering response may be frequency dependent, particularly if the particle size is close to the wavelength of the radiation (0.3 mm at 1 THz). Scattering causes particularly severe problems in THz-TDS, which measure the time domain THz signal and calculate the

⁵Retection is defined as 'the act of disclosing or uncovering something concealed' (Oxford University Press 1989)

5.7 Case Study #2: Powder Detection

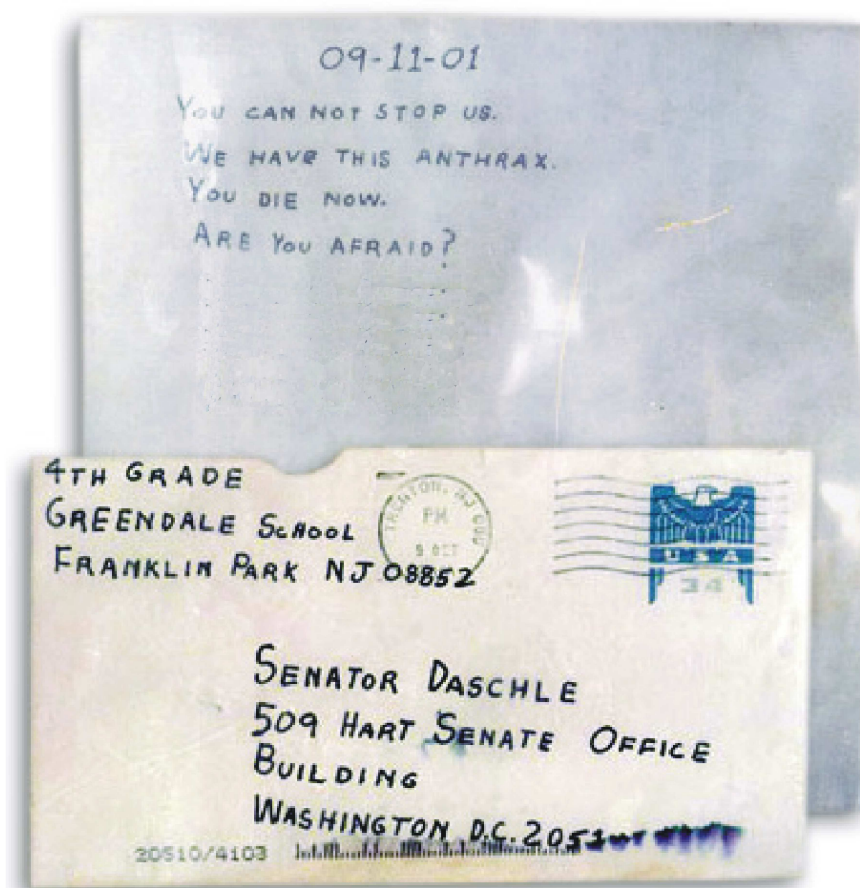


Figure 5.27. Photo of an envelope that contained *Bacillus anthracis* spores. The envelope was sent to US Senator Dreschler in 2001 and has been modified and reproduced from an FBI press release. After (Douglass 2003).

Fourier transform to obtain the spectral response. Multiple scattering paths distort the time domain waveform and may thereby obscure resonant absorptions in the frequency domain. Herrmann et al. (2002b) conducted a study in the identification of solid materials hidden in powders and demonstrated methods for distinguishing objects and measuring the powder density using THz-TDS. Kawase et al. (2003a) utilised a terahertz parametric oscillator-based spectroscopy system at 7 different frequencies between 1.3 THz and 2.0 THz to image samples of the illicit drugs methamphetamine and MDMA (*dl*-3,4-methylenedioxymethamphetamine hydrochloride) with an aspirin sample as a reference. The authors utilised measured amplitude spectra of the samples were used, together with the assumption that absorption dominated all scattering effects and the Wiener-Hopf equation described in Eq. (5.33) to accurately identify the

three powders from THz image data. This method was also extended to a quantitative estimation of powder concentrations based on THz images (Watanabe et al. 2004).

Due to the complexity of the problem, simple identification algorithms have had limited success in THz-TDS experiments and more complicated signal processing and machine learning approaches are favoured. This study applies the frequency domain techniques described in Sec. 5.3.3 to show that it is possible to classify powders concealed within envelopes despite the presence of strong scattering.

5.7.1 Data Acquisition

Preliminary Investigation

To investigate the applicability of THz imaging to the powder detection problem a simple test was performed using the chirped imaging system (Sec. 3.3.3) and the same method and algorithms described in Sec. 5.6 were applied.

Four different powdered samples: flour, salt, baking soda and seasoning, were attached to strips of tape and placed inside a paper envelope. The chirped probe THz imaging system was used to obtain an image. This took approximately 8 minutes to scan the envelope in 2 dimensions. The system may be improved to accelerate the image acquisition. Using a 1D chirped probe pulse THz imaging system (Jiang and Zhang 2000) it is feasible to attain a potential throughput of over 12 envelopes/minute. Approximately 800 milligrams of each of the sample powders were placed on double sided cellotape and attached to a piece of paper as shown in Fig. 5.28(a). The envelope was imaged and the transmitted THz waveform was measured at each pixel. Figure 5.28(b) shows a THz image produced by plotting the intensity of the THz pulse at a frequency of 0.3 THz, in Fig. 5.28(c) the classification algorithms based on second order FIR filter coefficients were used to differentiate between the different powders. The classifier was trained using the responses for 100 random pixels of each powder then the whole image was classified (Wang et al. 2002a).

This preliminary test indicated that THz systems have significant potential in mail screening applications. To more accurately assess the applicability of THz imaging to Anthrax detection a second preliminary test was conducted using samples of *Bacillus thuringiensis* (*B. thuringiensis*) bacteria. Several bacilli produce spores that are physically and chemically very similar to those produced by *B. anthracis*, including *B. thuringiensis*, which is commonly used for insect control in gardens and is non-pathogenic

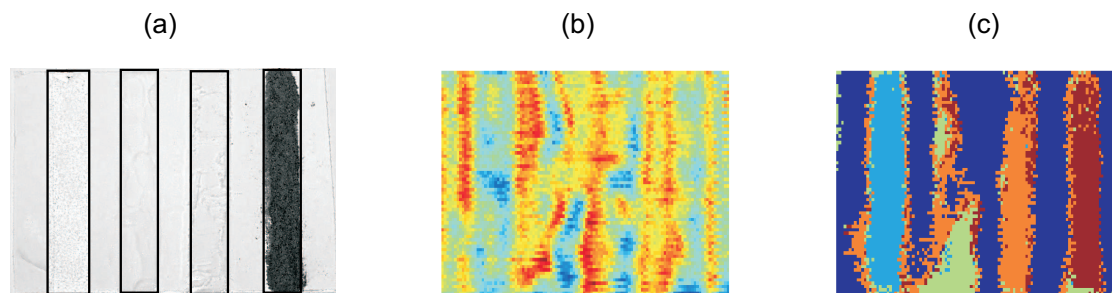


Figure 5.28. THz image of 4 different powders and classification results. (a) Optical image of a piece of paper containing samples of salt, baking soda, flour and Chinese five-spice seasoning (from left to right) 800 milligrams of each powder are spread on double sided cellotape. Another piece of paper was then stuck on top and the powders were placed in an envelope. (b) An image produced by taking the Fourier transform of the THz response at each pixel and displaying the amplitude at a frequency of 0.3 THz in a pseudo-colour image (red corresponding to maximum intensity, and violet to minimum intensity). (c) The results of classifying the THz data as described in the text. The image consists of five colours each corresponding to one of the five different classes: paper (dark blue), salt(light blue), baking soda (green), flour (orange) and seasoning (maroon). After (Wang et al. 2002a).

to man and other mammals. Genomic analysis has shown that several bacilli including *B. thuringiensis* and *B. cereus* have almost identical genetic makeup apart from the short sequence that codes the toxin (Ivanova et al. 2003). Approximately 500 milligrams of *B. thuringiensis* spore flakes were placed inside an envelope and imaged using the chirped probe pulse THz imaging system as described in Sec. 3.3.3. Figure 5.29(a) shows the envelope containing the *B. thuringiensis* spores and Fig. 5.29(b) shows the THz image of the envelope using the amplitude of the responses at 0.3 THz. The spores are clearly visible in the THz image. The second order FIR filter coefficients were calculated for each pixel in the image. Three classes were defined to describe the image, these were the empty envelope, the gum seal of the envelope and *B. thuringiensis* spores. A Mahalanobis distance classifier was trained using 50 pixels corresponding to each of these classes and then all the pixels in the image were classified. The results are shown in Fig. 5.29(c) and it is obvious that the bacterial spores are easily detected.

These two preliminary tests are encouraging and highlight the potential of THz imaging systems to the mail inspection application. These tests were conducted using a chirped probe pulse THz imaging system, which offers a high imaging speed but suffers a number of disadvantages as discussed in Sec. 3.3.3. Other authors have also

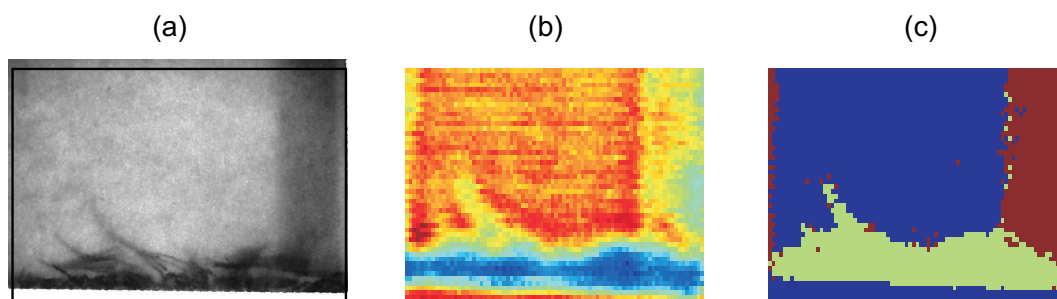


Figure 5.29. THz image of an envelope containing *Bacillus thuringiensis* spores. (a) Optical image of the envelope containing the spore flakes. The envelope is backlit to allow the spore flakes to be viewed. (b) THz image of the envelope containing the spore flakes. The amplitude of the responses at 0.3 THz were mapped to pseudo-colour (red corresponds to maximum amplitude, violet to the minimum amplitude). (c) The results of applying the classification algorithms described in Sec. 5.6. The second order FIR filter coefficients of 150 random pixels were used to train a Mahalanobis distance classifier and then all pixels in the image were classified. The image consists of three shades corresponding to the classified class of each pixel: blue (empty envelope), brown (envelope seal) and green (*Bacillus thuringiensis*).

demonstrated encouraging THz spectroscopic results for differentiating powders including bacterial spores (Choi et al. 2002, Watanabe et al. 2003). However the question of thickness-independent classification remains a concern. To investigate the capabilities of THz imaging more extensively a traditional scanned THz imaging system was used to consider samples of multiple thicknesses in the following sections.

THz Imaging System

A traditional T-ray imaging system based on the THz-TDS technique was employed. The system is described in detail in Sec. 3.3.1. A scanning delay line was used to offset the pump and probe beams and allow the temporal profile of the THz pulse to be measured. The sample was raster scanned in X and Y dimensions to acquire an image. This system offered high SNR but had a long acquisition time.

A 2 mm thick $\langle 110 \rangle$ ZnTe electro-optic crystal was used for the THz emitter and the THz field was generated via optical rectification of a 400 mW pump beam.

The THz beam was focused using parabolic mirrors to a spot size of 1 mm at the sample. The transmitted THz pulse was collected using parabolic mirrors and focused onto a 4 mm thick $\langle 110 \rangle$ ZnTe EO detector crystal. An optical chopper was employed

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to modulate the detected signal at a frequency of 182 Hz and a lock-in amplifier was used to detect the signal using a time constant of 10 ms. This system achieved a dynamic range in excess of 1,000 in electric field.

Powder Samples

The preliminary results with bacterial spores leads to the more general question of the ability of THz spectroscopy to detect specific powders given unknown (and variable) density, thickness and concentration. To attempt to investigate this problem multiple thicknesses of 7 different powders were imaged. The thickness of the powders were accurately controlled using the sample holder shown in Fig. 5.30. Approximately 10 grams of each powder were placed in a polyethylene plastic bag. Two teflon blocks were mounted on a manual translation stage that allowed the separation between the two blocks to be controlled. To test a given thickness of powder the teflon block spacing was set to provide the required gap (eg: 1, 2, 3, or 4 mm) and the plastic bag containing the powder was inserted between the teflon blocks. This ensured a relatively consistent powder density and accurate control over the powder thickness.

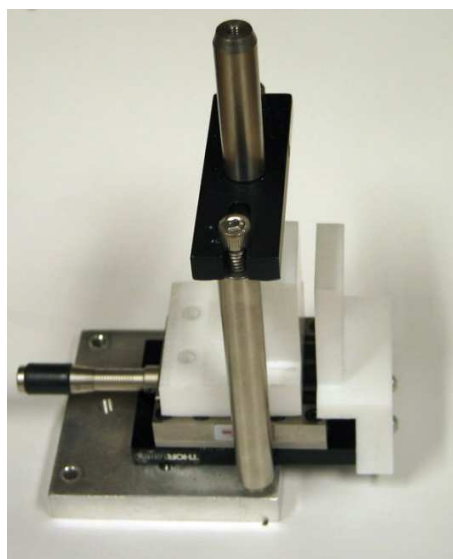


Figure 5.30. Photo of a teflon sample holder for powdered samples. One of the teflon blocks is fixed, while the position of the other is controlled using the manual translation stage. The gap between the two blocks may be adjusted to allow different thicknesses of powder to be considered.

The teflon sample holder was mounted on an X-Y translation stage and positioned in the THz beam. Teflon has a very low absorption coefficient at THz frequencies

and is dispersionless, allowing the THz pulse to propagate through the holder with minimal distortion. After a powder sample was inserted a 2D THz image of the sample was obtained. This image allowed the effects of differing scattering paths and minor variations in powder thickness and density to be observed. In general a 1D image was sufficient, and 50 pixel images (with a pixel spacing of 100 μm) could be acquired in under 30 minutes.

For this study 7 different powders were considered, these included: salt, sugar, powdered sugar, baking soda, talcum powder, flour and *Bacillus thuringiensis*. Each powder was imaged at 4 different thicknesses (1, 2, 3 and 4 mm) with the exception of *Bacillus thuringiensis* where the available quantity only permitted a thickness of 0.5 mm.

To test the ability of the classification system to detect powders inside envelopes, a composite target was constructed. This target consisted of thin layers of 6 different powders taped onto a piece of paper to form the letters 'THz.' Each section of the characters was formed using a different powder. The target was then placed inside an envelope and imaged using the THz imaging system. A coarse step size of 5 mm was used in the x and y dimensions and the THz time domain pulse was measured at each pixel. This image took approximately 5 hours to acquire. For practical mail inspection applications a faster THz imaging technique would be used, however this study allows the feasibility of THz inspection to be assessed. A photo of the target is shown in Fig. 5.31.

Data

The THz response of a powder may generally be characterised according to the frequency dependent refractive index, absorption coefficient and scattering properties of the powder. These depend both on the specific material and on the particle size of the powder (Pearce and Mittleman 2001). Figure 5.32 shows the time domain responses for several of the powders after transmission through 2 mm thick samples. The weakest signals are seen for the powders with larger particle size (sand and salt). For these powders the particle size is close to the wavelength of the THz radiation and results in strong scattering of the incident radiation. This is also evident in the frequency domain as demonstrated in Fig. 5.33.

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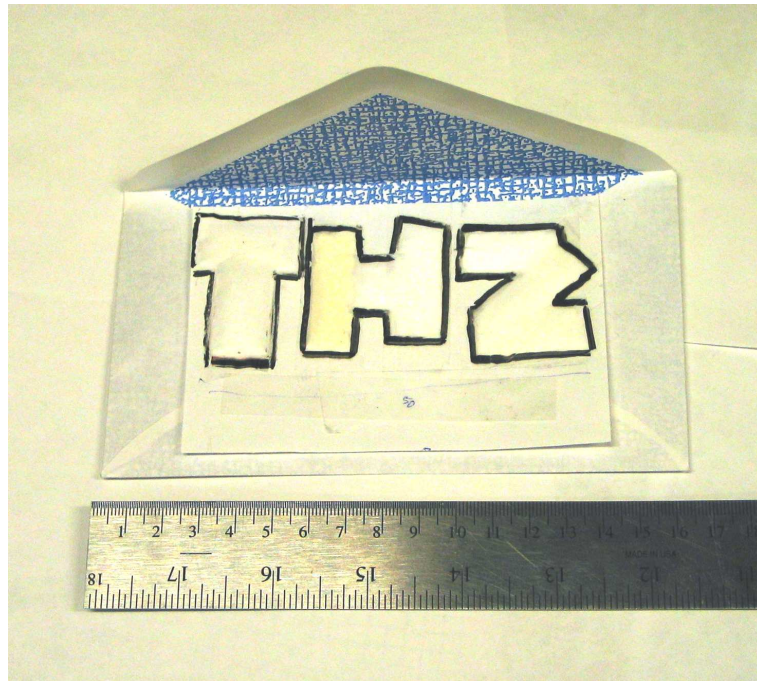


Figure 5.31. Photo of the powder target. The powders were taped onto a piece of paper to form the letters 'THZ'. The letter 'T' consisted of salt (upper) and sugar (lower), the letter 'H' consisted of flour (left) and powdered sugar (right and centre), and the letter 'Z' consisted of baking soda (upper) and talcum powder (lower and centre).

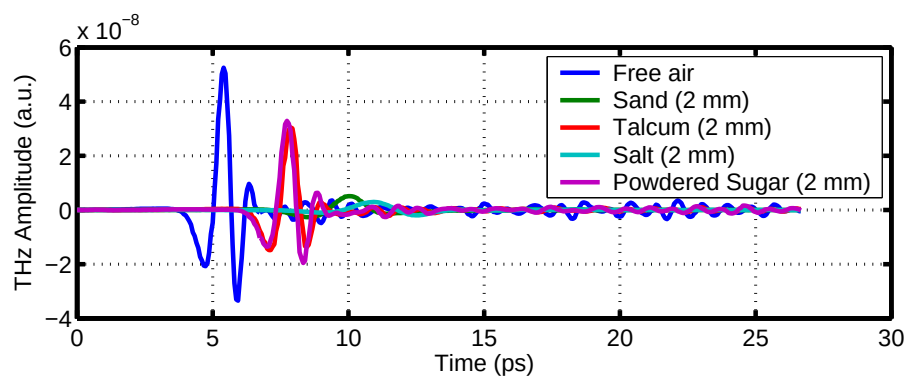


Figure 5.32. THz pulses after transmission through 2 mm of various powders. The powders with larger grain size (sand and salt) cause significant scattering of the THz radiation and the THz signal is attenuated compared with the response for the finer powders (talcum powder and powdered sugar).

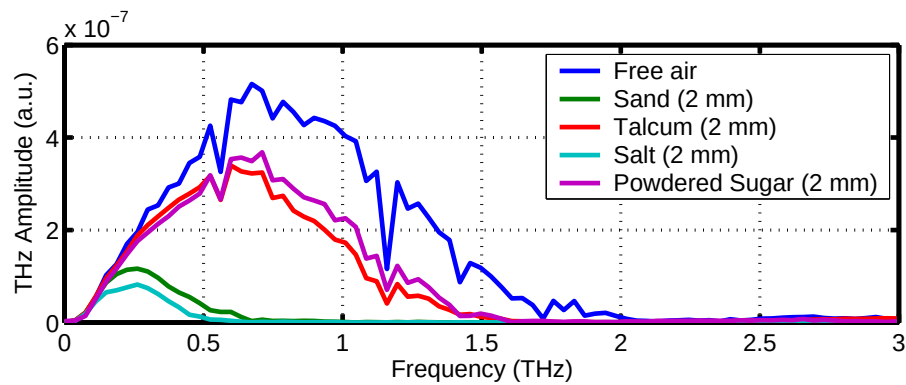


Figure 5.33. THz spectra after transmission through 2 mm of various powders. The absorption resonances at 0.56 and 1.16 THz are due to water vapour absorption.

As the thickness of the powders were varied the THz pulse showed an approximately linear increase in phase (or delay of the time domain pulse) and an exponential decay in amplitude with thickness. This is illustrated in Figs. 5.34 and 5.35 for flour of thicknesses 1,2,3 and 4 mm.

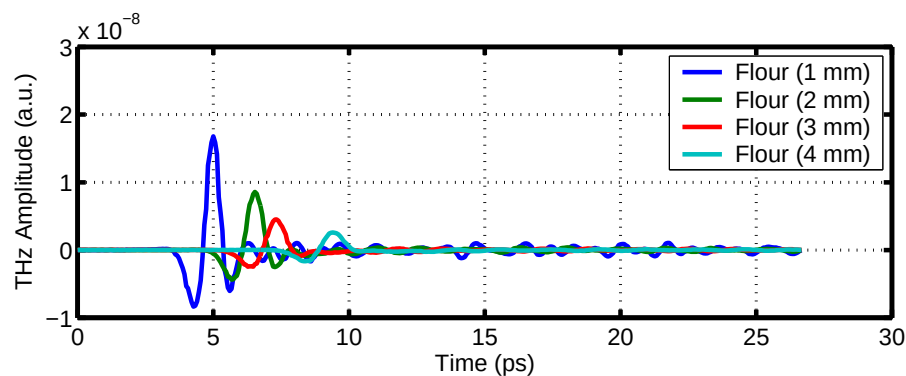


Figure 5.34. THz pulses after transmission through varying thickness of flour. Unbleached wheat flour was used. A linear relationship between the delay of the peak and the flour thickness is observable, while the amplitude of the THz peak varies exponentially with the flour thickness.

5.7.2 Classification

The data at the extreme thicknesses (1 mm and 4 mm) was used to train the Mahalanobis distance classifier described in Sec. 5.5. The accuracy of the classifier was then

5.7 Case Study #2: Powder Detection

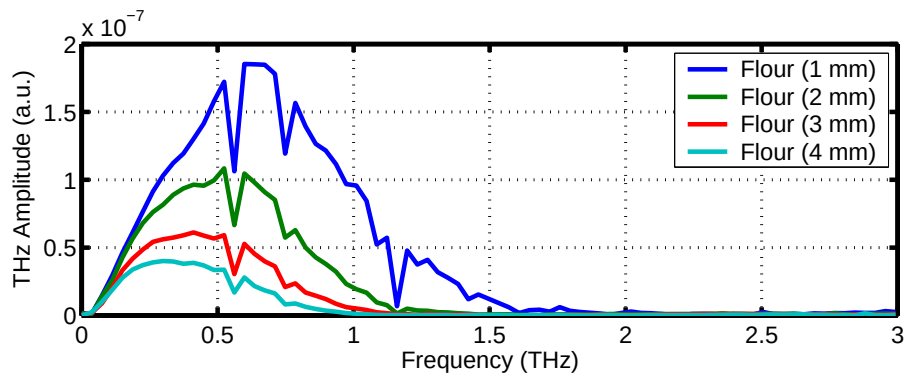


Figure 5.35. THz spectra after transmission through varying thickness of flour.

tested using the data for thicknesses of 2 and 3 mm. This tested the ability of the classifier to accurately generalise and classify powders at different thicknesses to those at which it was trained. This is obviously an important consideration in real-world detection problems.

The normalised, deconvolved frequency components were used as features for classification as described in Sec. 5.3.3. The first question addressed was the determination of the number of features (frequencies) required to ensure adequate classification performance. The genetic algorithm described in Sec. 5.4.3 was used to iteratively identify near-optimal combinations of frequency features. The genetic algorithm was modified slightly to allow the number of features used to remain constant from one generation to the next. An additional step was added to the crossover and mutation steps. The additional step compared the number of features selected in the evolved chromosomes and if it differed from the number in the previous generation, random bits were mutated until they matched. This ensures that the number of features, N , does not change over time. The parameters of the genetic algorithm were $p_{\text{mut}} = 0.01$ and $p_{\text{co}} = 0.7$. The termination criteria was after 50 generations, and the initial population consisted of 100 randomly chosen feature vectors.

To provide a visual indication of the separation of the classes, the results of 2D classification are shown in Fig. 5.36. The genetic algorithm was used to iteratively identify the optimal two frequencies for classification and frequencies of 0.41 and 0.6 THz were found to yield a classification accuracy of 87%. The normalised deconvolved amplitude for each powder at thicknesses of 2 mm, 3 mm and 4 mm are shown in Fig. 5.36. Each powder consists of three clusters in the 2D space; each cluster corresponding to a given powder thickness. The normalisation procedure serves to bring the clusters

closer together however they remain separated. In this case the training data is clearly far from normally distributed. However, it is anticipated that for more realistic training data acquired over a continuous range of powder thickness it *would* be normally distributed. The Mahalanobis distance classifier therefore remains a suitable choice for this application. In fact, a more complex classifier such as a neural network would likely define nonlinear decision planes around each cluster of the training data and would therefore be unable to generalise for powder thicknesses different to those in the training set.

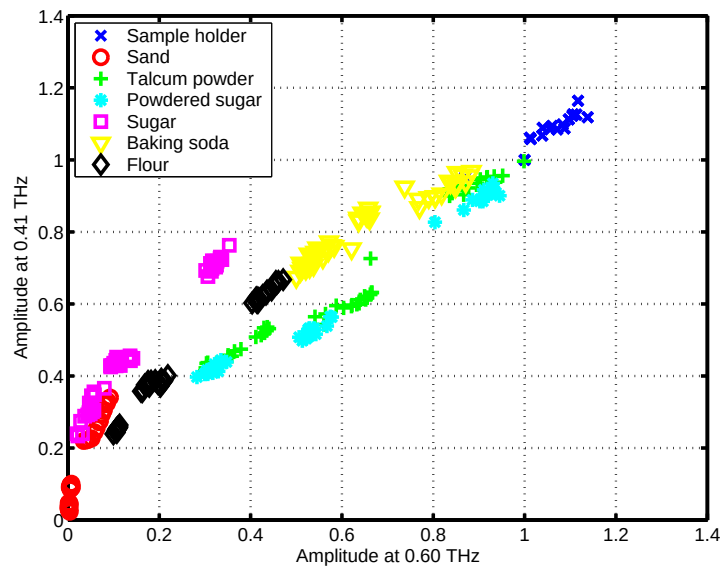


Figure 5.36. Scatterplot for powder data. The optimal frequencies for a two dimensional classifier were determined using the genetic algorithm procedure. Frequencies of 0.41 and 0.6 THz provided a classification accuracy of 87%. The amplitude scatterplot shows reasonable separation of the classes. The scatterplot shows the data for the 2 mm, 3 mm and 4 mm thicknesses of each powder. The high classification accuracy demonstrates that the classifier is able to achieve a degree of thickness-independent classification.

The genetic algorithm was then run iteratively for different values of N . The maximum classification accuracy after 50 generations was recorded and this procedure was repeated for $N = 1, \dots, 20$. The resultant maximum accuracy is shown in Fig. 5.37. For very low N there is insufficient information to allow a successful classification, however at $N = 8$, the classification accuracy plateaus at a near perfect level. Using $N = 8$ provided optimal classification accuracy and generalisation ability. The frequencies resulting in the maximal classification accuracy were: 0.30, 0.37, 0.60, 0.82, 1.42, 1.72,

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2.31, 2.43 THz. For larger N , the classification accuracy falls away as a result of the curse of dimensionality (see Appendix E).

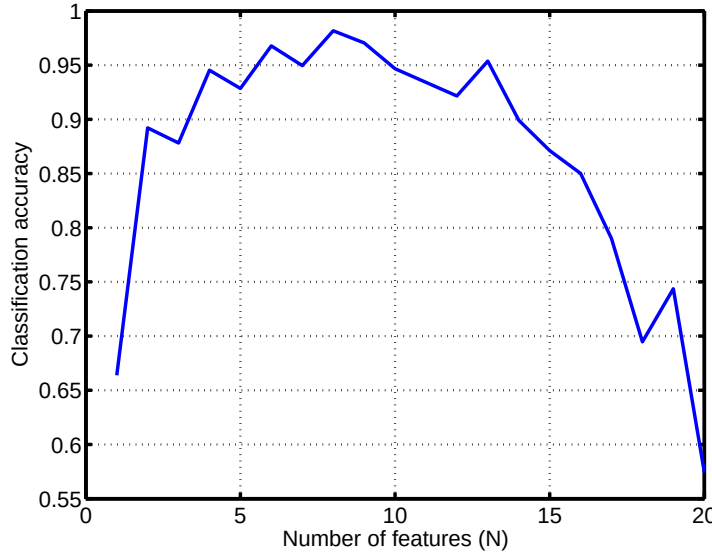


Figure 5.37. Plot of maximum classifier accuracy as a function of the number of features.

A Mahalanobis distance classifier was trained using N frequency components and then tested on a separate set of test data. The N frequency components were chosen using a genetic algorithm with $p_{\text{mut}} = 0.01$ and $p_{\text{co}} = 0.7$. After 50 generations of the genetic algorithm it was terminated and the maximum classification accuracy recorded. The classification accuracy was plotted and the process repeated for $N = 1 \dots 20$.

The *confusion matrix* for this classifier is given in Eq. (5.51). As described previously, the confusion matrix summarises the classifier performance. Each matrix element, $[i, j]$, shows the relative proportion of samples belonging to class i that were recognised as class j . The classes were empty holder(1), sand(2), talcum powder(3) powdered sugar(4), sugar(5), baking soda(6) and flour(7),

$$\begin{bmatrix}
 1.0000 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0.9216 & 0 & 0 & 0.0392 & 0 & 0.0392 \\
 0 & 0 & 1.0000 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1.0000 & 0 & 0 & 0 \\
 0 & 0.0098 & 0 & 0 & 0.9608 & 0 & 0.0294 \\
 0 & 0 & 0 & 0 & 0 & 1.0000 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 1.0000
 \end{bmatrix}. \quad (5.51)$$

Envelope Image Classification

This classifier was then tested on the envelope image shown in Fig. 5.31. This posed a more difficult classification problem because the paper, envelope and tape each provide additional distortions of the THz pulse. This therefore tests the ability of the classifier to generalise to real-world situations.

The classifier was trained using the 8 frequency components given above. All 4 powder thicknesses were used as training data. The envelope data was then deconvolved using a reference pulse measured through an empty envelope. A THz amplitude image is shown in Fig. 5.38. This image was generated by plotting the amplitude of the THz pulse in the time domain at each pixel. The letters are visible due to the increased absorption and scattering caused by the powders. The classification result is shown in Fig. 5.39. A grey-scale coded image is used to illustrate the classes assigned by the classifier to each pixel. The classes from darkest to lightest correspond to: empty envelope, sugar, salt, flour, powdered sugar, baking soda, and talcum powder.

A quantitative measure of the classifier accuracy in this test is difficult to define. However comparison of this image with Fig. 5.31 reveals that approximately 75% of the pixels of each powder are accurately classified.

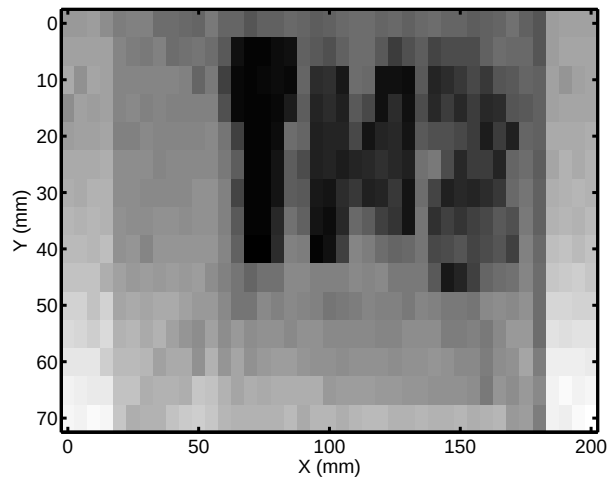


Figure 5.38. THz amplitude image of an envelope containing powders taped to form the characters 'THZ'. The image was produced using the amplitude of the THz pulses in the time domain.

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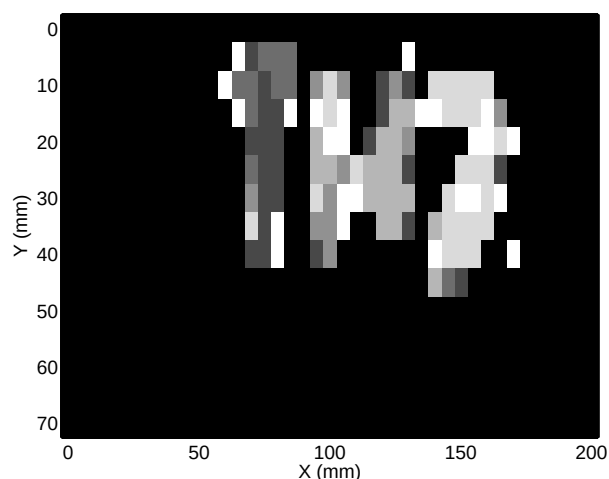


Figure 5.39. Classified image of an envelope containing powders taped to form the characters 'THZ'. The image was produced by classifying each pixel using a classifier trained with data for 6 different powders at thicknesses of 1,2,3 and 4 mm. The pixel is grey-scale coded according to the class assigned by the classifier. The image consists of 7 shades of gray. From darkest to lightest correspond to: empty envelope, sugar, salt, flour, powdered sugar, baking soda, and talcum powder.

5.7.3 Conclusion

The classification framework derived in the first half of this Chapter was demonstrated to allow THz pulsed imaging to successfully differentiate between unknown powders inside envelopes. The classification technique is robust to variation in the powder quantity and thickness. These simple feature extraction and classification algorithms allow for the automated analysis of THz images and may one day facilitate automatic detection of hazardous or illicit substances in mail and luggage using pulsed THz imaging. Wiener deconvolution and normalisation was used to calculate frequency dependent features for classification. The powder samples were classified using a Mahalanobis distance classifier. A genetic algorithm was used to iteratively refine a subset of the frequency components to use as feature vectors. This reduced the computational complexity of the classifier and improved its generalisation performance.

Limitations

The classification algorithms performed well on the data acquired in this case study. However, one of the major goals of any inspection system is its ability to detect the materials of interest in a wide range of real-world circumstances. This tests the ability

of the classification algorithms to generalise and obtain accurate results on data that does not satisfy the idealised conditions under which the case study data was acquired. For example this case study has not considered the effects of powder mixtures. If a powder of interest is mixed with another powder, the THz response will depend on each of the powders and their relative concentrations. In addition the density of the powders can have a significant effect on the THz response. For instance if a powder is crushed and the grain size modified, or compressed to form a pellet, then the frequency dependent scattering properties are dramatically altered (Markelz et al. 2000, Pearce and Mittleman 2001).

Figure 5.39 highlights the impact of less controlled imaging conditions on the classification accuracy. In this example the powder density and thickness were variable and the envelope and tape introduced additional distortions in the measured THz responses. The classification accuracy for this target was significantly degraded compared to the controlled single powder tests. Much improvement can be expected by simply collecting additional training data across the expected real-world variations. However, the extension of the developed classification framework to a perfectly general inspection imaging system is an open question complete with several challenges.

5.8 Case Study #3: Cancer Detection

T-ray imaging for medical applications is limited to the surface of the human body, for example for scrotal, corneal and dermatological/cutaneous imaging, but could find important use in estimating the depth of burns (Mittleman et al. 1999) and early warning signs of skin cancer. The level of image differentiation at these shallow depths is more precise than with the use of X-rays. Unlike X-rays, T-rays have the advantage of being a non-ionising radiation and thus represent a totally non-invasive diagnostic technique (Smye et al. 2001, Fitzgerald et al. 2002). Due to these significant advantages, cutaneous imaging for biomedical diagnostics is a significant application focus.

Terahertz systems have been proposed for a number of biomedical applications including the detection of tooth cavities (Ciesla et al. 2000) and burn severity diagnosis (Mittleman et al. 1999). A comprehensive review of terahertz applications in biology and medicine is provided in Siegel (2004). One of the most potentially significant biomedical applications is in the detection of skin cancers such as malignant melanoma and basal cell carcinoma. The incidence of these cancers continue to escalate and in the

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advanced stages of melanoma there is no curative therapy available (Altmeyer et al. 1997), early detection is therefore of prime importance.

Currently most dermatologists rely on a visual assessment of the patient for diagnosis. This diagnosis is not straight-forward and results in a large number of cases being treated inappropriately or inadequately. Hence there is considerable interest in the development of a non-invasive technique to improve clinician's diagnostic accuracy. Researchers have investigated the use of white light reflectance spectroscopy for this purpose (Wallace et al. 2000). They have found significant differences in the spectra for malignant and benign lesions, which may allow automated diagnosis. These studies have focussed on calculating metrics such as the tissue haemoglobin concentration, water concentration and haemoglobin oxygen saturation (Fishkin et al. 1997, Conover et al. 2000). A similar system based on the principle of THz time-domain spectroscopy has the potential to perform the same task with the added advantages of reduced Rayleigh scattering and finer frequency resolution.

5.8.1 Common Skin Cancer Indicators

Most forms of cancer are a result of the breakdown of cells' reproductive control mechanisms resulting in unmitigated growth. As a result a number of general detection methodologies have been proposed based on detecting one or more of the following markers:

- increased nuclear material, and increased nuclear to cytoplasmic ratio,
- increased mitotic activity,
- abnormal chromatin distribution,
- a progressive loss of cell maturity, as immature cells are proliferated, (Richards-Kortum et al. 1996)
- increased metabolic activity, and modified protein concentrations resulting from this activity,
- cellular crowding and disorganisation,
- increased vascularisation,

- specific changes in proteins, lipids, and nucleic acids located in the membrane, the cytoplasm and the nucleus of the cells and in the extra-cellular space. In particular increased fibronectin, and decreased collagen IV and laminin fragments in the extracellular matrix are considered indicative of melanoma (Yang et al. 1999).

5.8.2 Existing Techniques

Physicians commonly use a technique termed the 'ABCD system of melanoma detection'. This system is based on a visual (or digital image) inspection of suspicious moles and estimates the risk of melanoma using the four main indicators of asymmetry (A), border (B), colour (C) and dimension (D). This technique has been extended to infrared image analysis and it has been shown that low mean reflectance in the infrared and increased lesion size are indicators of melanoma (Bono et al. 1999).

A wide range of techniques have been developed for cancer detection using optical and infrared spectroscopic methods. Two of the most popular methods are optical fluorescence and Raman spectroscopy. Fluorescence spectroscopy measures the allowed electronic transitions of the sample while Raman spectroscopy measures the vibrational transitions from various molecules (Alfano and Katz 1996). Raman spectroscopy has very high spectral resolution and is capable of measuring the vibrational modes of molecules to yield 'molecular fingerprints' (Long 1977) that are highly specific to molecular structure. Raman spectroscopy has been shown to be sensitive to neoplastic change for many forms of cancer (Schrader et al. 1995, Lau et al. 2003) including the skin cancer basal cell carcinoma (BCC). Gniadecka et al. (1997) found that changes in the protein bands of amide I and amide III, amino acids proline and valine and lipid CH₂ vibrational modes were indicative of BCC growth. Raman spectroscopy is also able to determine concentrations of blood components and analytes in human sera (Berger et al. 1999, Qu et al. 1999).

Many parts of the infrared spectrum have been researched in the search for a reliable method of non-invasive cancer diagnosis. Near-infrared spectroscopy has been proposed using 4 or 5 different frequency bands of CW NIR light to detect areas rich in hypoxic blood, which indicates hemorrhaging resulting from accelerated tumour growth (Colak et al. 1999). A similar technique using Fourier transform infrared spectroscopy has shown promise in detecting oral squamous cell carcinomas (Fukuyama

et al. 1999), in assessing the clinicopathological grade of malignant lymphoma (Andrus and Strickland 1998) and has had marginal success in discriminating malignant melanoma (Weissman et al. 1997). Other techniques have focussed on detecting membrane protein change associated with cancer through the modified infrared spectra (Yang et al. 1999). Passive techniques have also been tested in the mid-infrared range of $250\text{--}430\text{ cm}^{-1}$ (Folberth and Heim 1984).

5.8.3 Far-Infrared Techniques

The most extensive study to date of the application of THz-TDS to cancer detection has been conducted by researchers at the University of Cambridge and TeraView Limited (Woodward et al. 2001, Woodward et al. 2002, Woodward et al. 2003). They have focused on basal cell carcinoma, a form of skin cancer, which seldom metastasises and is therefore not life-threatening, but can be disfiguring and is often misdiagnosed. Woodward et al. (2003) presents a clinical trial on excised (*ex vivo*) diseased and healthy tissue from 21 patients diagnosed with BCC. The excised tissue was imaged using a reflective mode scanning THz imaging system. A 20 Hz scanning delay line enabled an acquisition rate of 20 pixels/second and their quoted SNR was 6,000:1. The THz radiation was focused on the tissue samples and the reflected radiation collected using parabolic mirrors and detected using EO sampling. To differentiate between cancerous and non-cancerous tissue a technique termed *time post pulse* (TPP) was used (Woodward et al. 2002). In this method the THz signal is deconvolved using methods similar to those discussed in Sec. 5.2.4 and converted back to the time domain using the inverse Fourier transform. TPP normalises the response by dividing each sample by the peak in the time domain. TPP essentially quantifies the absorption and broadening of the THz pulse after reflection from the tissue sample. Figure 5.40 shows an example of the processing and results for a sample of healthy and cancerous tissue.

The work of Woodward et al. (2002) represents an important contribution to the development of a THz imaging system for clinical cancer detection. Here, 20 of the 21 samples considered were accurately diagnosed using the THz imaging results. They show that cancerous tissue results in increased absorption and broadening of the THz response. This change is attributed to “an increase in the interstitial water within the diseased tissue, or a change in the vibrational modes of water molecules with other functional groups.” (Woodward et al. 2003).

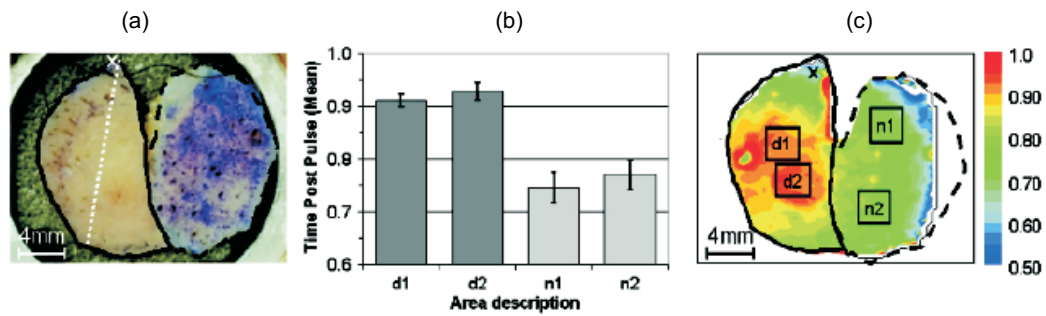


Figure 5.40. Analysis of excised cancerous tissue using THz-TDS. (a) Optical photograph of excised healthy dermal tissue and diseased (BCC) tissue from a patient. The normal tissue is shown on the right and is stained with ink for visual differentiation. (b) The tissue samples were imaged using a reflective mode THz imaging system and 2 regions were selected in each of the tissue samples. The THz responses were analysed as described in the text and the mean and standard deviation of the TPP values for the regions were calculated and plotted in the bar graph shown. (c) The THz image is shown by generating a pseudo-colour image based on the TPP value at each pixel. The cancerous and normal tissue can be seen to have differing TPP values. The regions selected for the plots shown in (b) are indicated by the square boxes. After (Woodward et al. 2003).

Other groups have investigated THz imaging of cancerous tissue (Knobloch et al. 2002). Löffler et al. (2001) showed that *dark* imaging, where only the portion of the illuminating THz radiation that is scattered beyond the ray path is detected, has promise in this context.

These previous studies have focused on excised tissue. In these cases a large number of factors influence the measured THz response, and changes in the concentration of water molecules and its bonds are likely to dominate the response. In this case study we sought to investigate the problem at a cellular level and isolate the cells' responses from that of bulk tissue properties.

Accordingly, THz spectroscopy was performed on human cells grown in culture. The cells were grown in transparent polystyrene flasks that enabled spectroscopic measurement of the live cells. The cells considered were normal human bone (NHB) osteoblasts and human osteosarcoma (HOS) cells. The classification framework developed earlier in this Chapter was then employed to allow automatic differentiation between the two cell types.

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5.8.4 Sample Preparation

The NHB cells were grown from patients undergoing a hip replacement. The cells were cultured from small pieces of trabecular bone for 4-6 weeks to obtain a confluent culture. The HOS cells were cultured from an immortalised cell line and a confluent culture was obtained within 1 week. The cells were cultured in 5 mL of Dulbecco's modified Eagle's medium (DMEM) supplemented with L-Glutamine (0.29 g/l), 10% foetal bovine serum and gentamicin (16 $\mu\text{g}/\text{ml}$) as an antibiotic. The same media was used for both types of cells to remove the possibility of different media influencing the results. Figure 5.41 shows a microscope image of each of the different cell types.

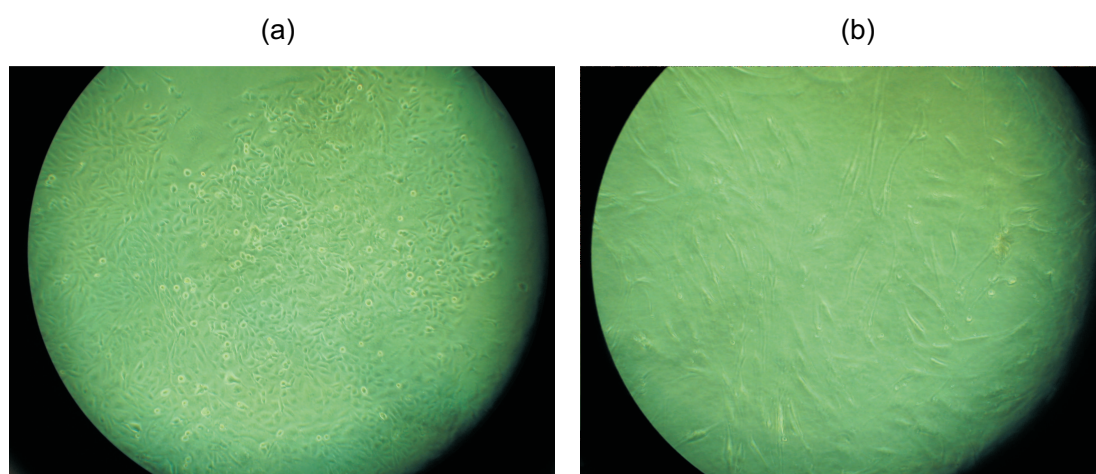


Figure 5.41. Normal and cancerous cells viewed under a microscope. (a) Human osteosarcoma cells. (b) Normal human bone cells. This image was taken several days before the spectroscopy results were obtained and the cells are not yet confluent.

The cells were cultured in 25 ml polystyrene flasks, in a 5% carbon dioxide environment at a temperature of 37°C. The cells form a thin layer attached to the bottom of the flask, and once they are 100% confluent they cover the entire bottom surface with a dense layer of cells. The flasks are transparent to THz radiation. To perform spectroscopy, the flasks were tipped on their side to allow the cell media solution to run off and the flasks were placed in the THz beam path as illustrated in Fig. 5.42. Three identical flasks were used. The first two contained confluent HOS cells and confluent NHB cells in cell media, having been incubated for 3 days to achieve a confluent culture. The third flask was used as a reference and contained only the cell media solution. A THz image was obtained providing spectroscopic information at 10 different positions, each separated by a distance of 50 μm . This was performed using a standard scanning THz

imaging system with a lock-in amplifier time constant of 10 ms. The image took less than 3 minutes to acquire. After this time the flask was removed from the spectroscopy system and reoriented to ensure that the cells did not die from lack of media.

This process was performed for each of the three flasks and then iterated a further 5 times thereby providing the THz response at 50 pixels for each of the flasks. This then provided sufficient data to allow statistical classification algorithms to be used to attempt to differentiate the cells.

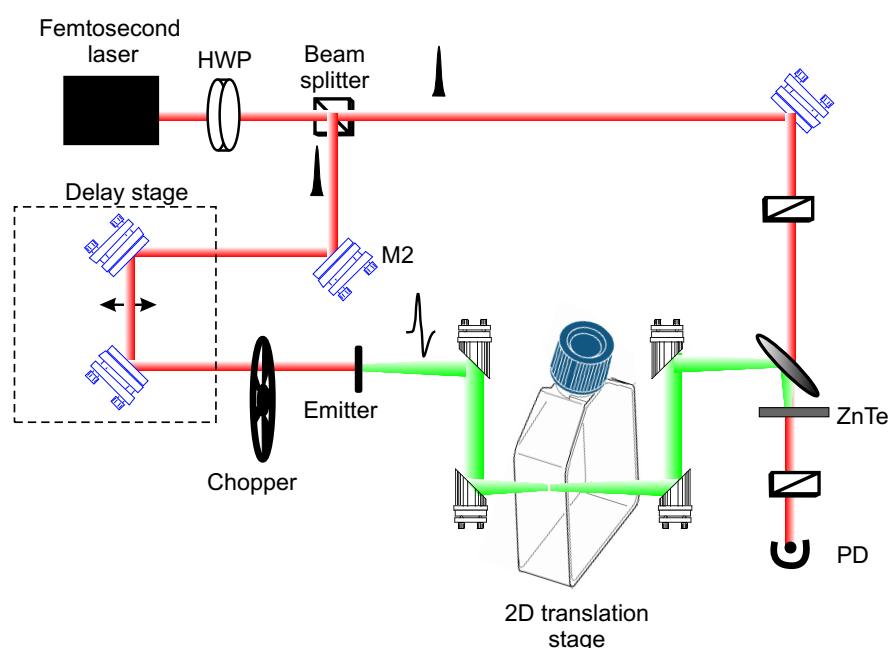


Figure 5.42. Scanned THz imaging system used to image cell flasks. The scanned THz imaging system is identical to the system described in Sec. 3.3.1. The cells are cultured in a polystyrene flask and a thin layer of cells grows on the bottom surface of the flask. The flask is tipped on its end and inserted into the THz beam such that the focal point of the parabolic mirrors is on the cell layer. The flask is raster scanned using a 2D translation stage.

5.8.5 Imaging Results

The average time and frequency domain responses of the three flasks are shown in Figs. 5.43 and 5.44. The error bars indicate one standard deviation either side of the mean for the 50 samples measured. From the THz spectrum it is clear that the cells result in additional absorption compared to the reference. However, the problem of

5.8 Case Study #3: Cancer Detection

distinguishing between the two types of cells is non-trivial because the difference between the two signals is less than the standard deviation (i.e. the noise level) of the data.

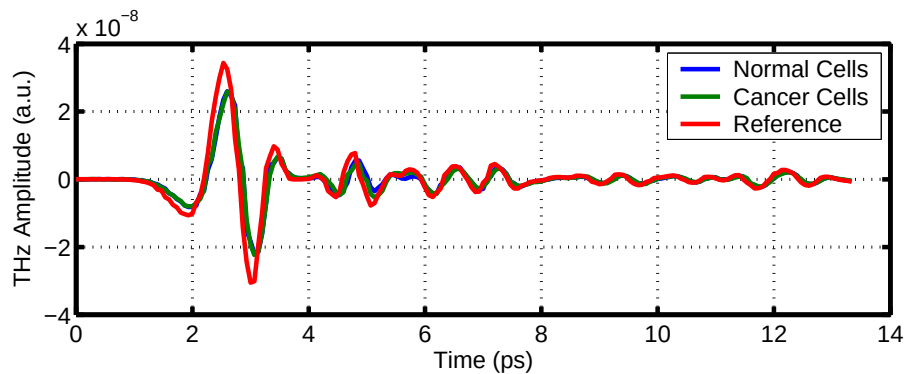


Figure 5.43. THz pulses after transmission through the cells. Three flasks were considered. One containing cultured normal human bone cells, another containing cultured human osteosarcoma and a third reference containing only the culturing Dulbecco's modified Eagle's medium (DMEM).

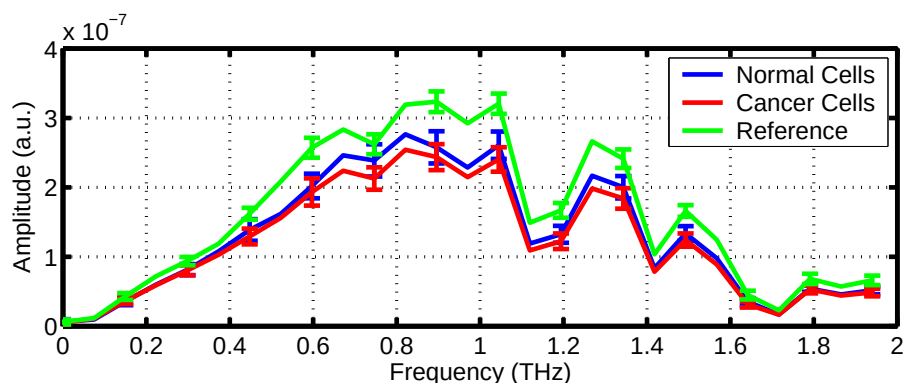


Figure 5.44. THz amplitude spectra after transmission through the three flasks. This plot shows the amplitude of the Fourier transform of the time domain pulses shown in Fig. 5.43. The error bars indicate one standard deviation either side of the mean.

Further understanding of the responses is provided by deconvolving the signals. The average response of the empty control flask was used as the reference for the deconvolution algorithm. Wiener deconvolution methods (Sec. 5.2.4) were used together with linearised phase unwrapping (Sec. 4.6.5) to obtain the frequency domain amplitude and phase response of the cells alone without the influence of the flask. These deconvolved responses are shown in Figs. 5.45 and 5.46. The normalisation stage described in Sec. 5.3.3 was *not* performed for this data. The normalisation procedure is useful

for classifying across data measured for different thickness samples, however in this study we are characterising cell layers of two different cell types. The thickness should not vary significantly for a given class and interclass thickness variation may prove a vital parameter for classification.

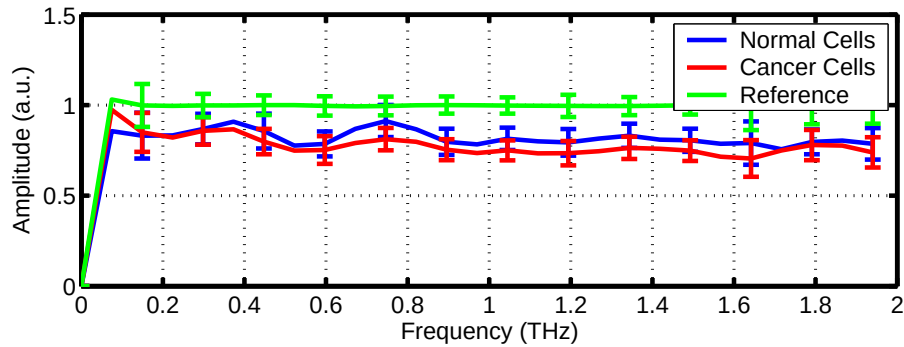


Figure 5.45. Deconvolved THz amplitude spectra for the three flasks. Wiener deconvolution was used to deconvolve all the cell responses using the average control flask response. The error bars indicate one standard deviation either side of the mean.

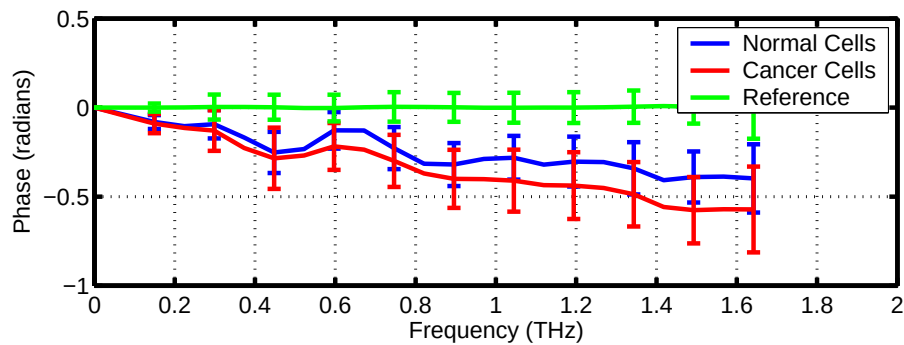


Figure 5.46. Deconvolved THz phase spectra for the three flasks. Linearised phase unwrapping was employed during the deconvolution procedure for the frequency 0-0.2 THz. The error bars indicate one standard deviation either side of the mean.

The cells do not have sharp resonant absorption peaks. This is expected for most solid materials, at room temperature, due to molecular collisions causing spectral broadening. However there is sufficient difference between the phase and amplitude responses to allow classification algorithms to distinguish between them.

5.8.6 Cell Classification

The Mahalanobis distance was used to classify the responses. The input features to the classifier were the deconvolved amplitude and phase at specific frequencies. It was not possible to manually choose optimal frequencies, so they were chosen using a genetic algorithm, which identified near-optimal frequencies. Half of the THz responses from each class were randomly selected and used as the training data set. The other 50% of the data was used to test the resultant classifier. The genetic algorithm used $p_{\text{mut}} = 0.01$ and $p_{\text{co}} = 0.7$. The termination criteria was after 50 generations, and the initial population consisted of 100 randomly chosen feature vectors.

The optimum training vector was found to consist of 6 frequencies: 0.22, 0.37, 1.12, 1.27, 1.34, and 1.57 THz. This provided a classification accuracy of 98.6% and a confusion matrix:

$$\mathbf{X} = \begin{bmatrix} 1 & 0.042 & 0 \\ 0 & 0.958 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (5.52)$$

This confusion matrix highlights the high classification accuracy of the algorithm. The only errors were ‘false negatives’, where cancerous responses were misclassified as normal cells. In a practical application a cost function would be incorporated in the classification algorithm to ensure that false negatives were less likely than false positives.

To visually illustrate the strength of this method, the genetic algorithm was programmed to choose the optimum 2 frequencies (note that this provides a poorer classification than using 6 frequencies as less information is available to the classifier, but it allows the results to be easily visualised). It determined that 1.00 THz and 1.57 THz provided a classification accuracy of 0.889. The scatter plots for both amplitude and phase at these frequencies are shown in Figs. 5.47 and 5.48.

The frequencies chosen by genetic algorithm were compared with two randomly chosen frequencies. The frequencies 0.52 THz and 2.00 THz were randomly chosen and the deconvolved amplitude and phase of the cell responses were used to train the Mahalanobis classifier. The scatterplots for both the amplitude and phase of the training data are shown in Figs. 5.49 and 5.50. The resulting classifier had a very poor accuracy of 0.670 when tested using 100 test responses.

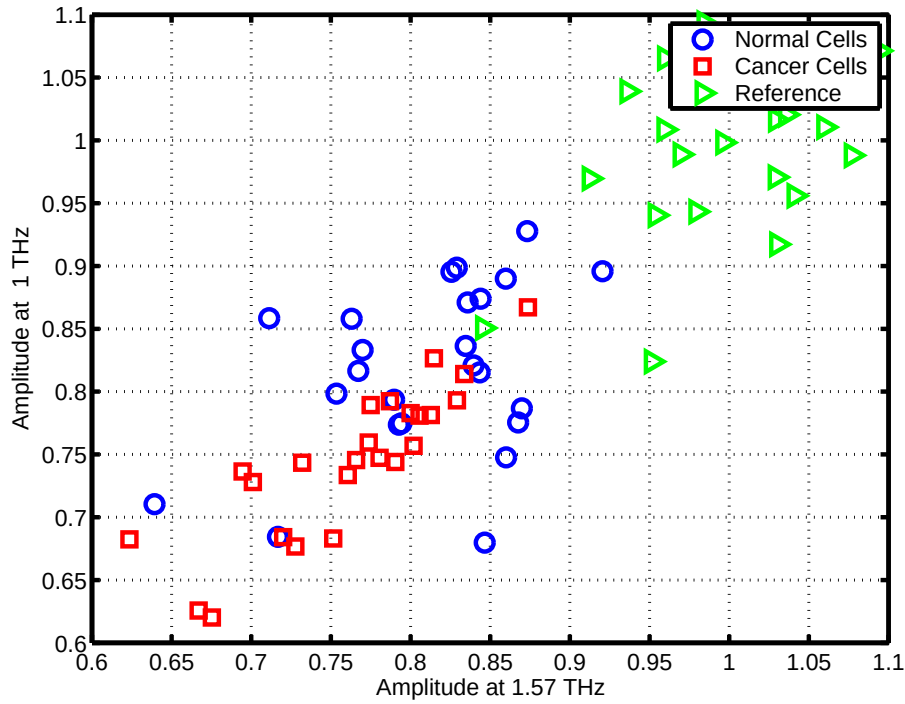


Figure 5.47. Scatterplot of the THz amplitude at the optimum two frequencies. The optimal 2 frequencies were found by a genetic algorithm to be 1.00 and 1.57 THz. The deconvolved amplitude of the cell responses are shown at these frequencies.

5.8.7 Comparison with Principal Component Analysis

A wide range of linear transforms are commonly employed for feature extraction from a data set. Perhaps the best known is principal component analysis, which is also known as the Karhunen-Loève transform. Principal component analysis calculates the eigenvectors and eigenvalues of the covariance matrix Σ for the data population. By ordering the eigenvectors in the order of descending eigenvalues, an ordered orthogonal basis is created. The first eigenvector is in the direction of largest variance of the data. Denoting the matrix containing the eigenvectors of the covariance matrix as $\mathbf{U}$, and each input vector as $\mathbf{x}$, gives

$$\mathbf{y} = \mathbf{U}(\mathbf{x} - \mu_x). \quad (5.53)$$

In the above equation μ_x is the population mean, and $\mathbf{y}$ is the vector $\mathbf{x}$ after transformation into the eigenspace. The eigenspace has the same dimension as the original data so no data reduction has been achieved, however the original data may be recovered exactly by the inverse equation,

$$\mathbf{x} = \mathbf{U}^T \mathbf{y} + \mu_x. \quad (5.54)$$

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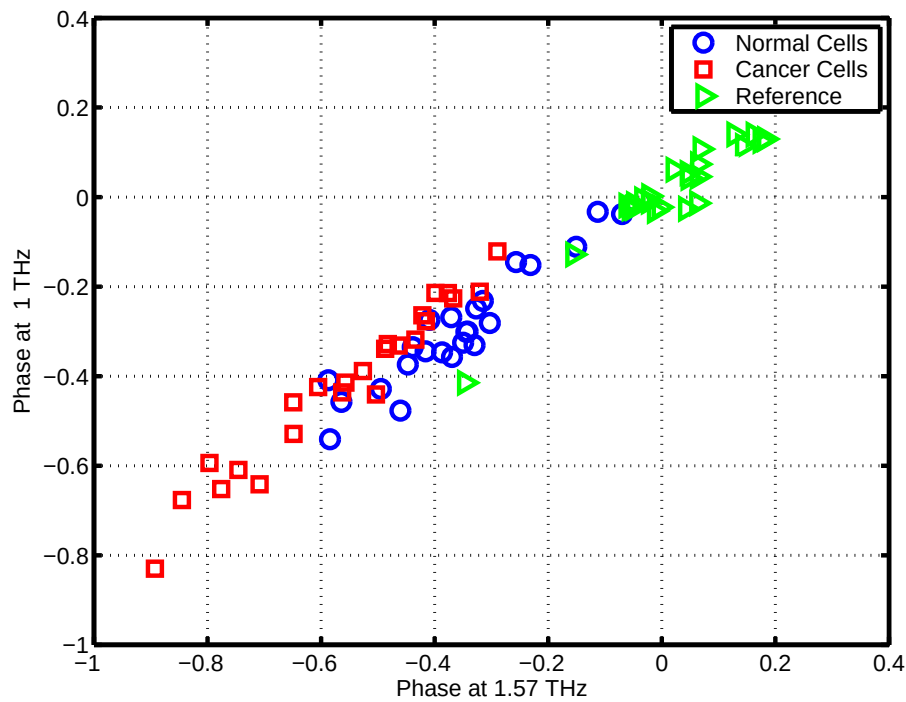


Figure 5.48. Scatterplot of the THz phase at the optimum two frequencies. The deconvolved phase of the human osteosarcoma (HOS) cells, normal human bone (NHB) cells and the reference flask are shown at frequencies of 1.00 and 1.57 THz. A Mahalanobis classifier was trained using this data and the amplitude data in Fig. 5.47. When tested on 100 random responses the classification accuracy was 0.889.

To compress the input data the first K eigenvectors are used to form a smaller dimensional space. The matrix containing the first K eigenvectors is denoted $\mathbf{U}_K$. Applying Eq. (5.53) with $\mathbf{U}_K$ results in a representation for x with K coefficients. Equation (5.54) may be used to recover a representation for x , which minimises the mean-square error between the representation and the actual value for a given value of K .

The Karhunen-Loève transform allows the dimensionality of the input data to be reduced while maximising the energy of the input data that is retained (Gonzalez and Woods 1992). This technique has been widely used for feature extraction in classification applications (Oja 1989).

To compare the performance of the feature extraction method developed in this Thesis with an established and widely used technique, principal component analysis based feature extraction was implemented and tested on the cell responses obtained in this case study. The same test and training data populations used in Sec. 5.8.6 were used. Instead of the pre-processing and deconvolution stages performed in Sec. 5.8.5, the

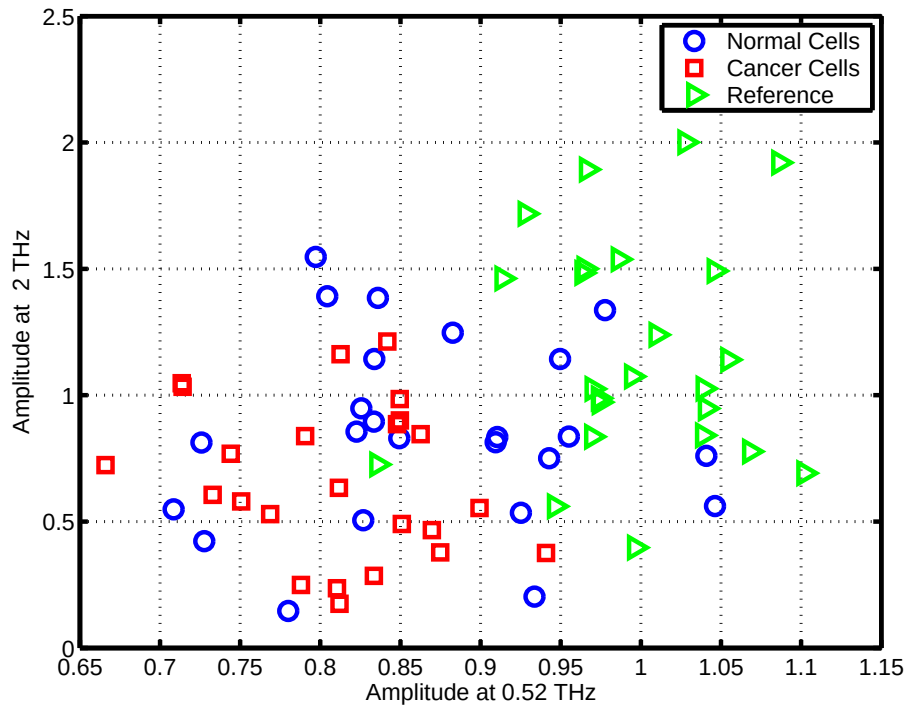


Figure 5.49. Scatterplot of the THz amplitude at two random frequencies. Two random frequencies (0.52 and 2.00 THz) were chosen and the deconvolved amplitude at these frequencies are plotted for the HOS and NHB cells and for the reference flask. There is poor separation between the two types of cells.

covariance matrix Σ and mean μ responses were calculated using the time domain THz signals of each of the three classes combined. The eigenvectors of the covariance matrix were calculated. Figure 5.51 shows the first three eigenvectors for the cell data. The first 10 eigenvalues are shown in Fig. 5.52. These values are plotted in a log scale for clarity. The magnitude of the eigenvalue relates to the variance of the data set in the direction of the corresponding eigenvector. It can be seen that the first eigenvalue accounts for the majority of the signal energy.

The first 12 eigenvectors were then used to define a feature extraction technique. Equation (5.53) was applied to each of the THz responses with $\mathbf{U} = \mathbf{U}_{12}$. This provided 12 coefficients representing each THz response. The training data set was used to train a Mahalanobis distance classifier, which was then used to classify the test data set in exactly the same manner as adopted in Sec. 5.8.6. Then, 12 eigenvectors were used to allow a direct comparison with the results in Sec. 5.8.6, where 6 frequencies were

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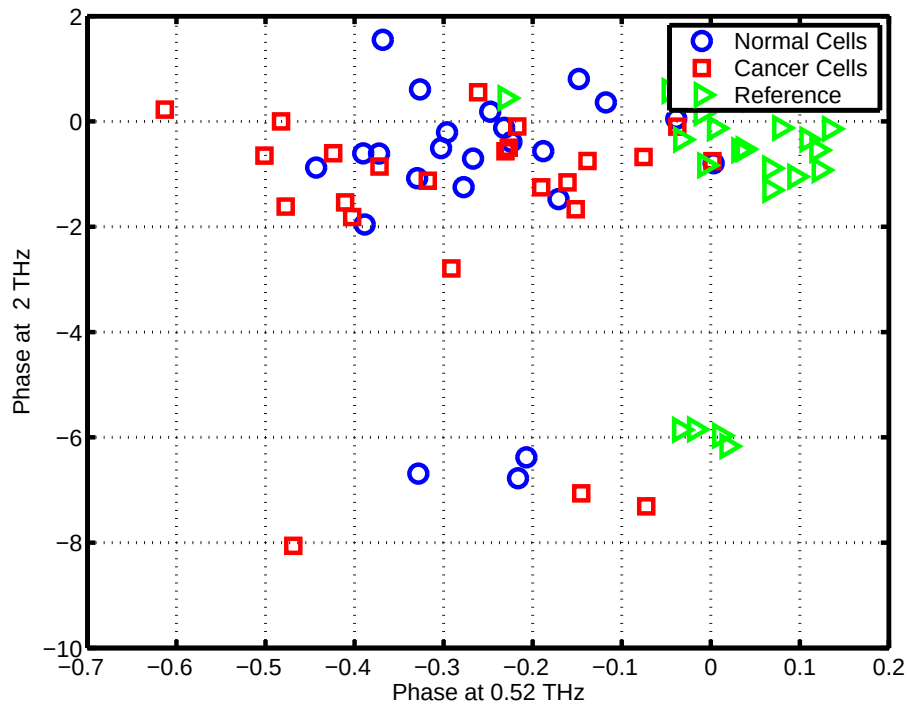


Figure 5.50. Scatterplot of the THz phase at two random frequencies. The deconvolved phase of the HOS and NHB cell responses are plotted at the randomly chosen frequencies of 0.57 and 2.00 THz. As with the amplitude data there is a poor separation between the two classes. A Mahalanobis distance classifier was trained using this data and the amplitude data shown in Fig. 5.49 and tested on a separate set of responses. The classifier yielded an accuracy of 0.670.

chosen and the deconvolved amplitude and phase at each frequency were used as coefficients. The principal component analysis based classifier resulted in a classification accuracy of 83.3% and a confusion matrix of

$$\mathbf{X} = \begin{bmatrix} 0.667 & 0.125 & 0 \\ 0.292 & 0.875 & 0 \\ 0.042 & 0 & 0.958 \end{bmatrix}. \quad (5.55)$$

These results are clearly inferior to the results shown in Sec. 5.8.6. This result is not unexpected. Principal component analysis is optimum for data compression and performs well in classification applications where the inter-class differences are significantly higher than the intra-class variation. However, in this application there are only subtle differences between the classes and the random variations within the classes are significant, as seen in Figs. 5.43 and 5.45. In this case, principal component analysis is

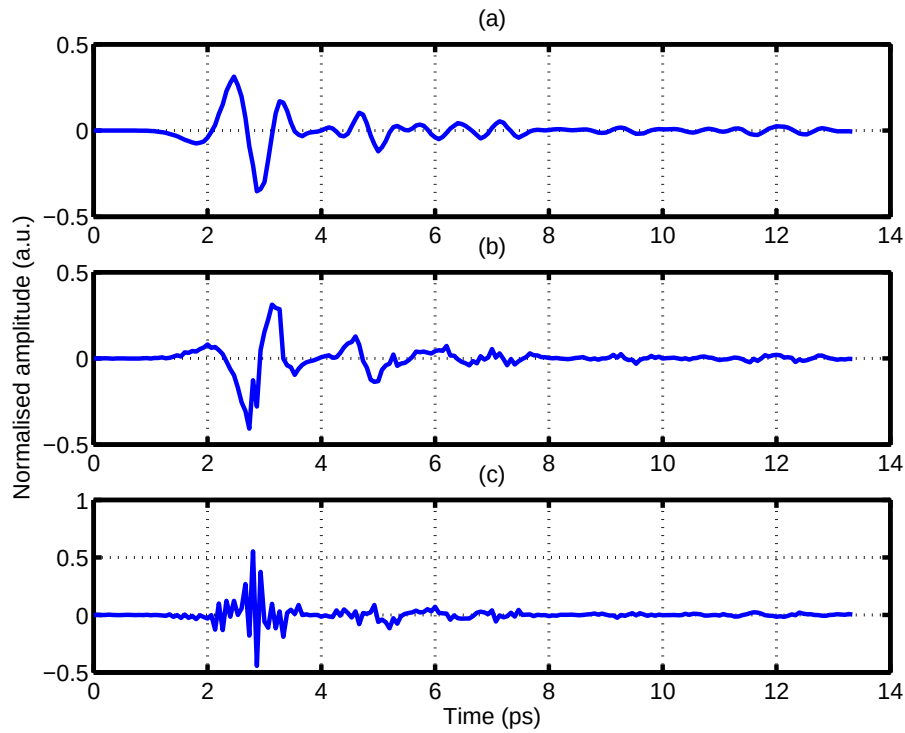


Figure 5.51. Eigenvectors of the covariance matrix for the cellular THz responses. The covariance matrix for time domain THz pulses was calculated. The eigenvectors of this covariance matrix were then calculated and ordered by descending eigenvalue. The first eigenvector describes the direction of maximum variance in the THz responses. The first eigenvector is shown in (a), the second in (b) and the third in (c).

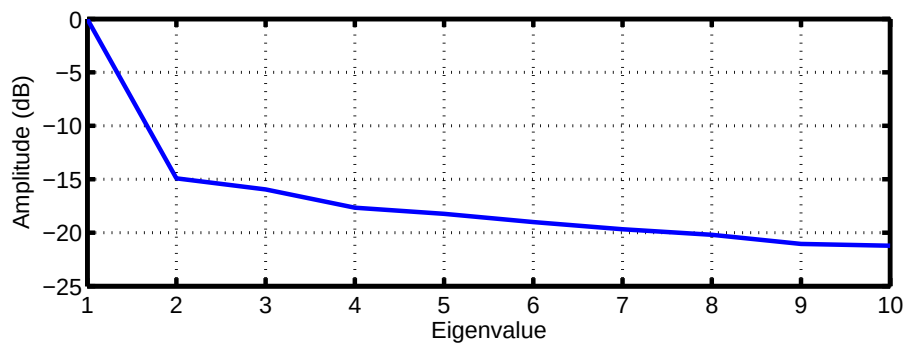


Figure 5.52. Eigenvalues of the covariance matrix for the cellular THz responses. This figure plots the first 10 eigenvalues corresponding to the eigenvectors shown in Fig. 5.51. The eigenvalue magnitude is shown in dB for clarity as the first eigenvalue is over 100 times greater than the 10th.

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not optimal for classification and techniques that infer additional information from the problem domain offer improved performance.

To illustrate this fact, Figs. 5.53 and 5.54 show scatter plots for the THz responses after projection onto the first 4 eigenvectors. Figure 5.53 shows the results of projection onto eigenvectors 1 and 2. While eigenvector 1 provides reasonable segmentation of the classes (potentially due to differences in the time domain amplitude), eigenvector 2 adds little to the classification performance (this can be seen by considering the projection of the data shown in Fig. 5.53 onto the two axes). Eigenvectors 3 and 4, as shown in Fig. 5.54, provide very little differentiation between the three classes.

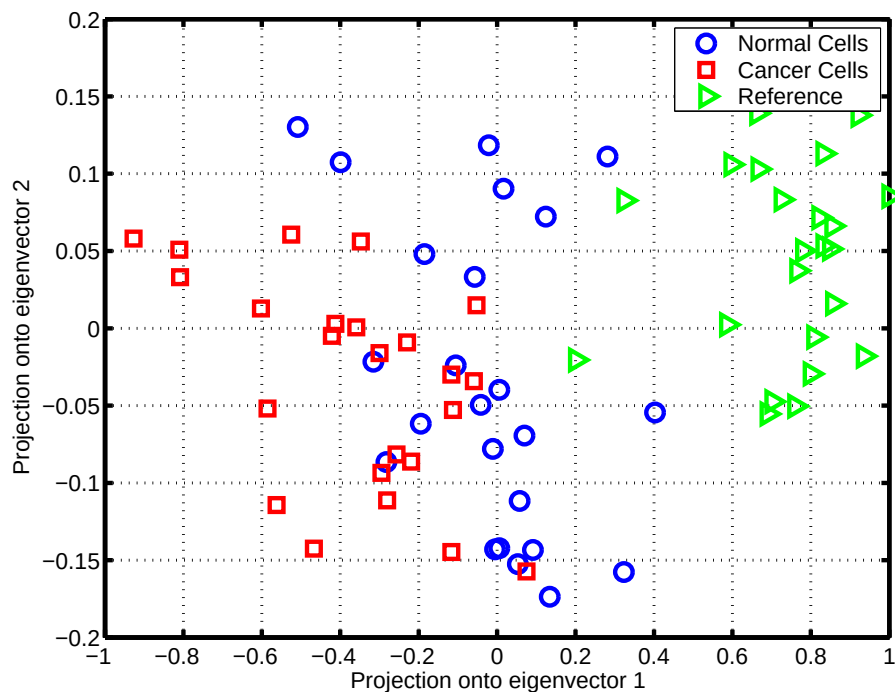


Figure 5.53. Scatterplot of the projection of the THz responses onto the first two eigenvectors. Equation (5.53) was used to project the THz responses onto a 12 dimensional eigenspace. This figure shows the results in the first 2 dimensions. Eigenvector 1 provides a reasonable differentiation between the 3 classes.

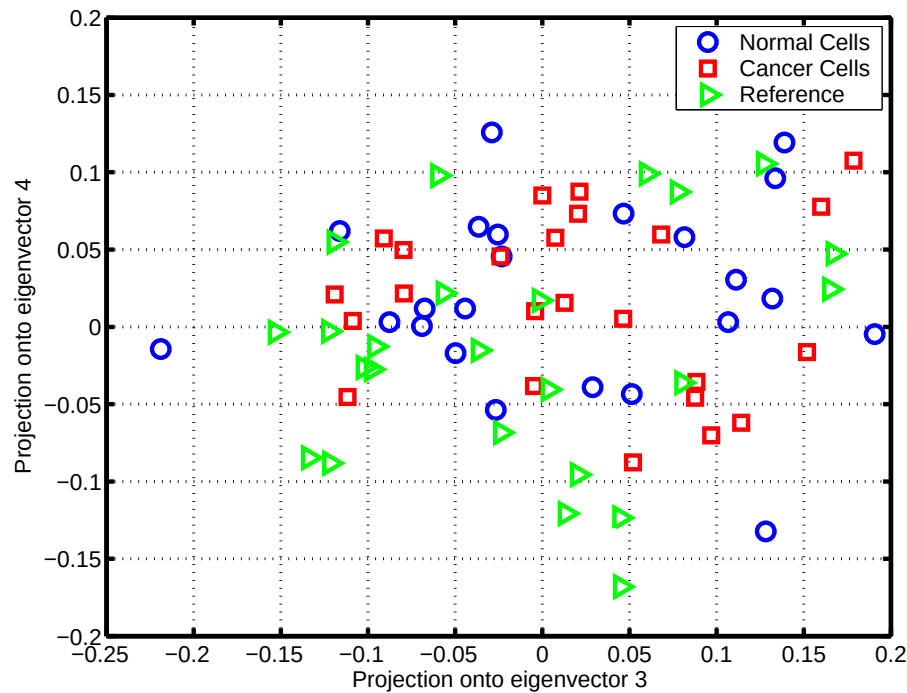


Figure 5.54. Scatterplot of the projection of the THz responses onto the third and fourth eigenvectors. Equation (5.53) was used to project the THz responses onto a 12 dimensional eigenspace. This figure shows the results in dimensions 3 and 4. There is no visible segmentation between the three classes. This highlights one of the disadvantages of applying PCA for feature extraction: the directions of maximum variance are not necessarily related to inter-class differences.

5.8.8 Conclusions and Future Directions

The results of this preliminary case study are promising. They show that THz-TDS can detect the response of a thin layer of cells with a thickness of under $100\ \mu\text{m}$. They also show that there is sufficient spectral signature information to allow a classifier to be trained to recognise specific types of cells. One potential explanation for the detectable difference between the cells is the different production of extracellular matrix by the two cell types. Osteoblasts secrete abundant type I collagen-rich matrix, whereas osteosarcoma cells usually produce less matrix.

This would appear to be a significant result, however a number of questions remain to be answered. As with the previous study the most significant problem is transitioning the results from the meticulously controlled environment of a case study to a more general setting. This study only considered one flask of each cell type. Further

5.8 Case Study #3: Cancer Detection

work is required to confirm the results and conclusively show that the detected differences are in fact due to the cellular responses and not other potential experimental variations such as long term laser drift, variations in flask thickness and degree of cell confluency. More exhaustive trials should be able to establish this fact by culturing several flasks containing each of the cell types and obtaining THz data using multiple THz-TDS systems.

It is also important to verify that the observed classification accuracy can be maintained in the presence of standard environmental variations. These include the relative humidity, the specific THz emitter and detector characteristics and the concentration and type of cell media solution. Similar experiments should be conducted with other cell types, particularly skin cancer cells cultured *in vitro* to investigate the scope of THz-TDS in cellular identification.

A further issue that must be addressed in the future relates to the resolution of THz-TDS. With a focal diameter of greater than 1 mm the THz spectral response is averaged over an extremely large area relative to the size of the cells under investigation. In the IR band microspectroscopic techniques are available, and are capable of acquiring spectral responses with a spatial resolution of 18 μm . This is sufficient to differentiate between the response of a cell nucleus and cytosol (Diem et al. 2000, Diem et al. 2002, Gazi et al. 2003). Lasch et al. (2002) studied skin fibroblasts and sarcoma cells and concluded that previous FTIR results identifying spectral lines corresponding to cancer (Andrus and Strickland 1998, McIntosh et al. 1999) may instead be due to differences in the cells' divisional and metabolic activity rather than signatures specific to cancer. FTIR microspectroscopic studies have also been performed to identify a host of potentially obscuring variables in screening for cervical cancer (Wood et al. 1998). It was demonstrated that leukocytes, endocervical cells, seminal fluids, thrombocytes, bacteria and nylon threads all exhibit spectral responses that can potentially obscure the response of cervical malignancies. Similar problems are likely to hinder *in vivo* THz cancer diagnosis.

Raman spectroscopy can also be performed with high spatial resolution using a confocal microscope. A goal of Raman microspectroscopy is the development of a Raman fiber-optic needle device capable of insertion in the human body and *in vivo* cancer diagnosis with high resolution. This has particular application in breast cancer diagnosis (Shafer-Peltier et al. 2002).

5.9 Chapter Summary

The intention of the three preliminary case studies outlined in this Chapter was to provide a motivational setting for THz material identification. The promising results obtained are, by nature, preliminary and do not allow strong conclusions to be drawn. However, these results do highlight the potential of THz spectroscopy and of the classification algorithms employed. These case studies also serve to illuminate key open questions to be addressed in future large-scale studies. A pattern recognition framework for material identification with THz imaging systems has been developed. This framework incorporates preprocessing, feature extraction and classification methods specifically tailored for the THz imaging domain.

Wavelet denoising is near optimal for denoising nonstationary or pulsed signals such as THz waveforms. An experimental study was performed to demonstrate the performance of wavelet denoising, to compare the available wavelet basis and identify strong candidates for this application. Wiener deconvolution was also evaluated for THz preprocessing. Wavelet denoising was shown to be capable of improving the signal to noise ratio of the measured THz signals by almost 30% (Ferguson and Abbott 2000).

Two feature extraction techniques were developed to reduce the dimensionality of the acquired THz image data. These techniques allow efficient and accurate classification to be performed. An adaptive system identification problem was formulated to allow a material's THz response to be parameterised as a linear filter. By restricting the order of the filter, the filter taps provide an efficient representation of the material response. Second order finite impulse response filters were shown to accurately represent the response of a range of materials when imaged using a chirped probe THz imaging system. The high classification accuracies resulting from this model indicate that it may have correlation with the underlying physical model. This issue warrants significant future attention.

A more intuitive feature selection method is to simply choose frequencies at which molecular resonances manifest for the materials of interest. Variations on this method work well for gas identification with THz spectroscopy due to the presence of clearly identifiable and theoretically predicted resonant frequencies. Unfortunately for solids the THz spectra are seldom so gracious, and instead consist of a multitude of weak, thermally broadened spectral lines that prohibit manual identification of frequencies

of interest.⁶ Accordingly an artificial intelligence system using a genetic algorithm was constructed to select appropriate frequencies. The THz spectral responses were deconvolved using Wiener deconvolution, normalisation algorithms were applied, and the deconvolved frequency components were selected using a genetic algorithm. The fitness function for the genetic algorithm was the classification accuracy over a representative set of test data and thus incorporated a measure of the generalising ability of the resultant classifier.

A Mahalanobis distance classifier was shown to be a good match for the THz data statistical properties. It also allowed the performance of the feature extraction methods to be accurately compared without requiring fine tuning of weights or basis functions.

With the pattern recognition framework in place, three case studies were conducted in material identification with THz imaging. These studies focused on important potential applications of THz imaging in biological tissue identification, mail screening for bacterial spores and cancer detection. Preliminary ‘proof of concept’ experimental tests were conducted in each of these application domains and the results processed using the developed algorithms. Promising results were revealed in each case study, a critique of the results was presented, and future directions were highlighted. The first ever experimental results demonstrating THz-TDS based imaging of bacterial spores and *in vitro* cultured cells were presented.

The case studies in this Chapter have focused on processing 2D THz data, however the classification framework is generic and may be expected to provide similarly promising results when applied to 3D THz data reconstructed using the techniques presented in Ch. 4. However, current 3D imaging systems impose severe limits on the acquisition speed and SNR as a result of their relative immaturity. Future research in improving these aspects of 3D imaging and the application of classification algorithms to 3D image data is likely to prove extremely fruitful.

⁶Cooling the sample to liquid nitrogen temperatures and below, to reduce spectral broadening, is a possible future approach.

Chapter 6

Conclusion

THZ imaging technology has advanced to the point where practical commercial systems are now feasible. With this advancement has come the potential for 3D tomography and spectroscopic functional imaging. Each of these techniques have significant promise for future applications. Combined they offer a powerful tool for industrial inspection, security screening and biomedical imaging.

This Thesis has developed systems and algorithms for both THz tomographic imaging and THz material identification. It has discussed improvements to traditional 2D THz imaging in order to provide the necessary speed and SNR for advanced applications. These imaging systems were used to design three unique tomographic imaging techniques and the capabilities and advantages of each technique were presented. A classification framework was developed for material identification based on THz spectroscopic data and this framework was demonstrated in three case studies drawn from promising application fields. Combined, these tools pave the way for the development of 3D THz inspection systems with broad applicability.

This Chapter concludes this Thesis by drawing together the research described in previous chapters and discussing future directions for continued development in this domain.

6.1 Introduction

“... nothing tends so much to the advancement of knowledge as the application of a new instrument. The native intellectual powers of men in different times are not so much the causes of the different success of their labours, as the peculiar nature of the means and artificial resources in their possession.”

- Sir Humphrey Davy, 1840

6.1 Introduction

Section 6.2 summarises the research conducted in this Thesis and describes the major conclusions and novel contributions of this work. Section 6.3 then highlights a number of remaining open questions identified in the course of this research and details research areas which form the logical next steps to build upon the contributions of this Thesis.

6.2 Thesis Summary

This research aimed to advance THz inspection systems in two main areas: 3D tomographic techniques, and material identification. The Thesis is logically divided into these two topics. A third subdivision arose to support each of these topics: the advancement of existing 2D THz imaging systems. The Thesis conclusions are presented in these three categories.

6.2.1 THz Imaging Systems

Chapter 3 reviews the current state-of-the-art in THz imaging and surveys the current opportunities and limitations in the field. It then describes in detail the three pulsed imaging architectures that were utilised in this research.

Traditional scanned THz imaging is based on THz-TDS and dates back to Hu and Nuss (1995). It represents the most established and probably the most commonly used THz imaging technique due to its high SNR, and simple setup. The system used in this Thesis utilised a regeneratively amplified Ti-sapphire laser and alternate THz sources to meet the particular experimental requirements. The need to

raster scan the target and scan the delay stage makes this system the slowest of the three techniques considered, but its SNR is unrivalled, exceeding 1,000. The imaging system is described in detail and example images presented in Sec. 3.3.1.

THz imaging using 2D FSEOS offers many potential benefits over scanned imaging.

The need to raster scan the target is removed and near real-time THz imaging is feasible. However, this method distributes the available THz power over all pixels and removes the LIA and therefore results in a significant reduction in SNR. Additionally the inhomogeneities inherent in large ZnTe crystals result in distortion of the THz image.

Typically dynamic subtraction is utilised to improve the SNR of 2D FSEOS by canceling the $1/f$ noise from the ultrafast laser. In this technique (Sec. 3.3.2) the optical chopper is synchronised with the $f/2$ subharmonic of the CCD sync output. For a low pulse repetition frequency regeneratively amplified laser dynamic subtraction has limited benefit due to the lack of synchronisation with the laser output. To correct this problem a synchronised dynamic subtraction technique was developed (Sec. 3.3.2). This technique allows the chopper and CCD to be synchronised to the laser timing reference. This results in a significant improvement in the image SNR as demonstrated in Ch. 3.

Synchronised dynamic subtraction allows the THz modulated optical field to be measured with high accuracy. However a true image of the target is only obtained in the ideal case where the probe beam, the residual birefringence of the sensor crystal and the incident THz field (in the absence of a target) are independent of sensor position. In practice all of these parameters vary. A sensor calibration algorithm was developed to deconvolve the influence of system inhomogeneities from the recorded images. This simple technique significantly improves the image quality and allows the system to accurately record THz images of low contrast targets such as polyethylene.

THz imaging using a chirped probe pulse represents a recent addition to the available THz imaging techniques and promises to allow terahertz imaging and spectroscopy to extend to new applications in the monitoring of ultrafast phenomena through its capacity for single shot measurements. The first ever transmission mode images measured using this technique are presented in Ch. 3.

The chirped imaging technique allows the full THz temporal response of a single pixel to be measured simultaneously. This has advantages over other THz imaging techniques in that if the sample moves during a scan the signature responses of the pixels are not corrupted, only the pixel to pixel intensity may change.

The chirped imaging architecture is described in detail and a mathematical model presented allowing an approximation to the THz spectra to be extracted from the chirped probe measurements. The chirped probe imaging system benefits from the synchronised dynamic subtraction and sensor calibration techniques described in Sec. 3.3.2. Experimental results are presented demonstrating the performance of the imaging system and its limitations.

These three imaging systems form the basis of the tomography systems presented in Ch. 4 and were used to obtain the data presented in the case studies in Ch. 5.

6.2.2 T-ray Tomography

Chapter 4 presents the major technical contributions of the Thesis with the development of three novel THz tomography systems. Imaging architectures, reconstruction algorithms and experimental results are presented for each.

T-ray holography builds on recent work in THz time-reversal imaging (Ruffin et al. 2001) and Kirchhoff migration (Dorney et al. 2002). Two dimensional FSEOS THz imaging was used to construct a T-ray holography system and the system was tested, initially on simple 2D targets.

Young's traditional double slit experiment was recreated using THz radiation and backpropagation of the Fresnel-Kirchhoff equation was used to recover the geometry of the slits with high accuracy. Importantly for generalised inspection applications, the distance to the target was not known *a priori* but was independently estimated by the developed reconstruction algorithm.

An expression for the resolution of the technique was derived and shown to be dependent upon the size of the sensor crystal, the distance to the target and the frequency of the radiation.

This 2D holography system offers an increase in acquisition speed of several orders of magnitude over previous migration and time-reversal techniques. This

speed increase is provided by the 2D FSEOS imaging system. The results demonstrate that targets can be accurately reconstructed using the limited aperture presented by the sensor crystal.

The 2D system was then extended to allow 3D images of point scatterers to be reconstructed. A novel reconstruction algorithm was developed utilising the windowed Fourier transform. This algorithm was successfully demonstrated in imaging point scatterers located in two well-separated planes. Figure 6.1 reproduces the reconstructed results of the 3D T-ray holography system.

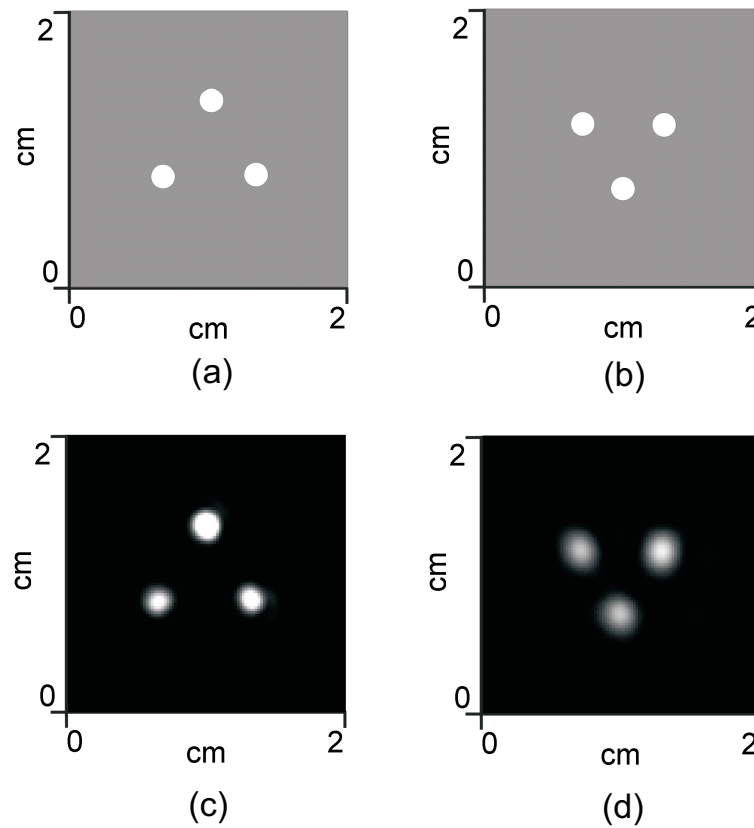


Figure 6.1. Schematic of holography target samples and their reconstructed holograms. (a) Schematic of sample S_1 , (b) Schematic of sample S_2 , (c) Reconstructed hologram of S_1 , (d) Reconstructed hologram of S_2 . This figure is reproduced from Ch. 4. For further details see Sec. 4.4.

T-ray holography is not without its limitations. Its extension to more general targets presents significant challenges and it provides only qualitative images. However, the image fidelity is high and it can acquire images extremely quickly.

6.2 Thesis Summary

T-ray diffraction tomography is based on approximations to the Helmholtz equation, which describes electromagnetic wave propagation in general media. Unlike T-ray holography, which utilises the Huygen-Fresnel diffraction equation and is therefore best suited to point scatterers in free-space, T-ray diffraction tomography is applicable to more general targets.

The first order Born and Rytov approximations to the Helmholtz equation assume that the scattered field is small compared to the incident field and are therefore applicable to low contrast targets. They allow simplified solutions to the Helmholtz equation to be derived via the Fourier Diffraction Theorem. This derivation is presented in Sec. 4.5.

The resultant reconstruction algorithms require the diffracted THz field to be measured along a receiver array for multiple diffraction angles. A diffraction tomography system was constructed using the 2D FSEOS THz imaging system by mounting the target on a rotation stage 50 mm from the sensor crystal. Several test targets were imaged and the validity limits of both the Born and Rytov based reconstructions were investigated. The Rytov approximation was found to be less restrictive and a 3D reconstruction was performed on a target consisting of three rectangular cylinders. The results are reproduced in Fig. 6.2.

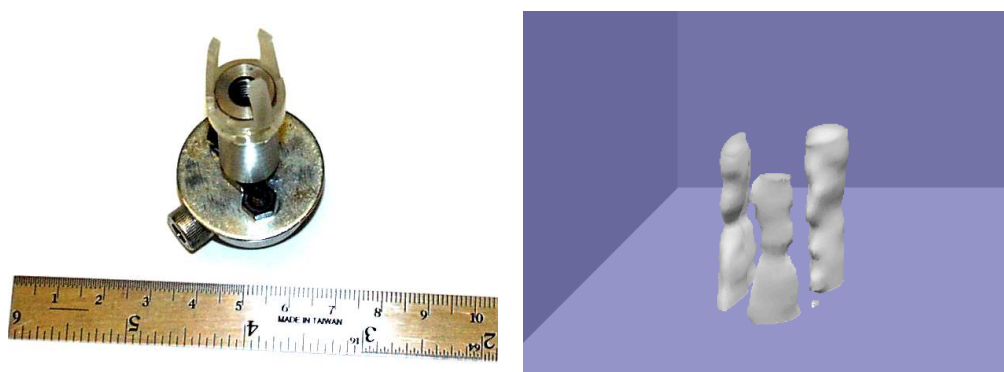


Figure 6.2. A test structure imaged by the T-ray DT system and reconstructed result. (left)

The target consisted of 3 rectangular polyethylene cylinders. (right) Each horizontal slice was reconstructed independently and combined to form a 3D image. The reconstructions were thresholded at 50% of the peak amplitude and surface rendered. This figure is reproduced from Ch. 4. For further details see Sec. 4.5.

T-ray diffraction tomography was demonstrated for spectroscopic 3D imaging and the limits of applicability of the technique were investigated.

T-ray computed tomography represents the culmination of this research on 3D imaging systems. It provides spectroscopic 3D images with high fidelity. The Rytov approximation to the Helmholtz equation was adopted to derive a series of experimental conditions under which the filtered backprojection algorithm (familiar from X-ray CT applications) may be utilised to reconstruct targets based on the measured THz field. The following two requirements were found:

1. the target's lateral extent in the direction of the THz wave vector is less than the Rayleigh range of the THz beam, and
2. within the Rayleigh range the THz beam propagates as a planar Gaussian wave.

Based on these requirements an architecture was designed using a focused THz beam. A slow 2D tomography system was developed based on scanned THz imaging. This system provided long acquisition times but very high SNR and image quality. Several test targets were fashioned from polystyrene and used to characterise the system. A interpolated cross-correlation algorithm was developed to estimate the phase shift of the THz pulse after transmission through dispersionless targets and this algorithm was utilised as part of the reconstruction algorithm.

The resolution of the T-ray CT system was measured and found to be better than 0.5 mm, clearly illustrating the power of this coherent tomography technique. T-ray CT was used to recover the frequency dependent refractive index of polystyrene with high accuracy. Figure 6.3 reproduces the results of the 2D T-ray CT system for a polystyrene test target.

A high acquisition speed 3D T-ray CT system was then developed based on THz imaging with a chirped probe beam. This system was demonstrated for 3D imaging of a turkey femur and various test targets. The ability to differentiate between different materials based on their refractive index was demonstrated.

T-ray CT is a novel extension of terahertz time-domain spectroscopy with numerous potential applications. It has been used to extract the frequency dependent refractive index of a 3D target thereby providing spectroscopic images of weakly

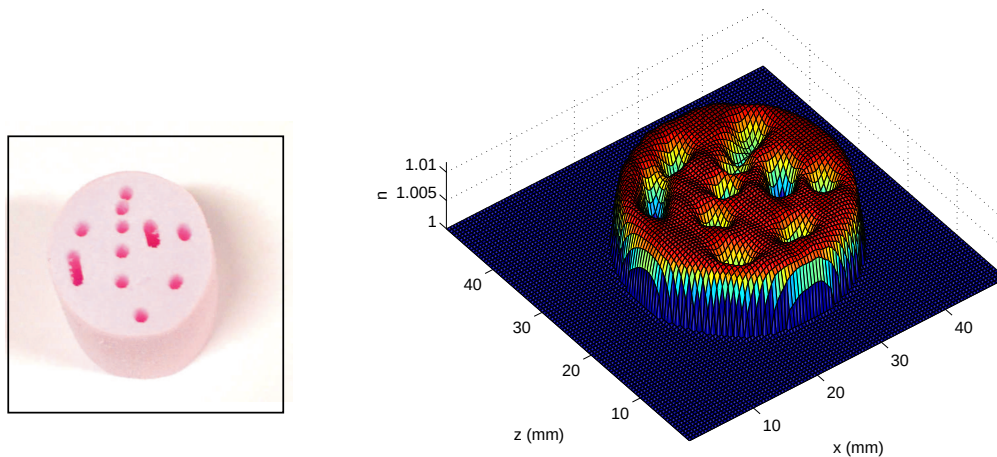


Figure 6.3. Detailed polystyrene resolution test target and its reconstruction. (left) 2 mm diameter holes were drilled into a polystyrene cylinder with varying interhole distances. (right) 3D visualisation of the reconstructed cross section of the test target. This figure is reproduced from Ch. 4. For further details see Sec. 4.6.

scattering objects. T-ray CT provides the refractive index of the sample without requiring *a priori* knowledge of the sample thickness and allows the internal structure of objects to be revealed.

6.2.3 Material Identification

Chapter 5 develops a classification framework for the identification of materials in pulsed THz images. The classification framework consists of three major parts: pre-processing, feature extraction and classification. A number of techniques are proposed and investigated in each section.

Preprocessing describes the task of attempting to isolate the material information present in the THz waveforms from systematic and random noise sources present in the data. Wavelet denoising and Wiener deconvolution are demonstrated for this purpose. Wavelet denoising is known to be near-optimal for pulsed signal processing due to their time-frequency localisation. The available wavelet families are investigated to experimentally identify the optimal wavelet basis for THz denoising. The Coiflet order 4 wavelet was shown to outperform the other bases and to significantly outperform stationary techniques such as Wiener filtering.

Wiener deconvolution is used to suppress the noise amplification problem commonly encountered in THz pulse deconvolution.

Feature extraction is used to reduce the dimensionality of a classification problem to yield more efficient classifiers with higher generalisation performance. Two feature extraction schemes are described in Sec. 5.3. The first uses low order linear filters to model the THz response of the material in a system identification formalism. The finite impulse response filter coefficients were shown to accurately model material responses for a range of different materials.

The second feature extraction method used a genetic algorithm to adaptively identify THz frequencies of interest. The deconvolved THz amplitude and phase were used as features. A normalisation stage was added to allow thickness independent material classification. The fitness function for the genetic algorithm was the classification accuracy over a test population, ensuring that the genetic algorithm chose features with good generalisation properties.

Classification algorithms abound, and are a fruitful research topic in a range of disciplines. For this application a simple Mahalanobis distance classifier was used. This classifier was chosen as it displays near-optimum properties for a wide class of input data, does not require fine tuning of classifier parameters, and is relatively robust to overfitting problems.

With a classification framework established, the remainder of Ch. 5 turns its attention to three topical case studies investigating the potential of THz spectroscopy in different application settings. Experiments were conducted and the data processed using techniques from the classification framework to attempt to identify specific materials in THz images.

Case study #1: Tissue identification. The first case study considered tissue samples of beef, chicken muscle and chicken bone, imaged using the chirped probe THz imaging system. The FIR filter coefficients were used as feature vectors and the Mahalanobis distance classifier demonstrated high classification accuracy.

Case study #2: Powder detection. The second case study focused on the contemporary problem of the detection of bacterial spores inside envelopes and discrimination between spores and benign powders. Preliminary studies were conducted

6.3 Future Directions

demonstrating the potential of THz imaging in this arena. Samples of several different powders were then imaged over multiple thicknesses to investigate the application of the developed classification framework to thickness independent classification. Promising results were obtained.

Case study #3: Cancer detection. The final case study aimed to complement recent work on the detection of basal cell carcinoma tissue using THz spectroscopy. To isolate the cellular response of cancerous cells from the multitude of complicating factors encountered in *in vivo* studies, an *in vitro* approach was adopted. Normal human bone cells and osteosarcoma cells were cultured in polyethylene flasks. Once confluent the cultures were imaged using a THz imaging system and the spectra analysed under the developed classification framework. Once again, the results were promising and form a foundation for future in-depth studies.

In all three case studies high classification accuracies were demonstrated. These studies highlighted the performance of the classification tools developed in Ch. 5, but they are, by nature, preliminary. Rather than attempting to perform comprehensive studies in these application areas, these studies sought to highlight the potential of THz inspection systems and to provide a basis for future work.

6.3 Future Directions

With any rapidly developing technology there are a vast number of open questions and promising future research problems. THz inspection systems are no different. This section surveys the scope of the future work in this area and particularly highlights promising extensions of the work presented in this Thesis.

THz Imaging

Much of the progress in THz spectroscopy systems in the last 20 years is attributable to progress in THz sources and detectors, and these remain core areas of development. THz imaging systems will benefit greatly from future high power THz sources such as the quantum cascade laser and others discussed in Sec. 2.1. Higher power sources, coupled with high sensitivity detectors will result in higher SNR and faster acquisition speed THz imaging systems. Section 3.2.2 details several of the most pressing limitations of current THz imaging systems. Future research will continue to push forward

on each of these fronts. In particular THz imaging systems will continue to increase in speed, bandwidth and resolution, while reducing in size and cost. The goal of a T-ray endoscope remains elusive but promises significant benefits, especially in biomedical imaging.

The importance of reflection-mode imaging will continue to grow due to the high absorption of many materials in the THz band. THz gene chips (Nagel et al. 2002), skin cancer imaging systems (Woodward et al. 2002) and non-destructive testing are just a few of the applications that will drive future THz research.

THz Tomography

Three dimensional THz imaging is an active research area and recent progress is very encouraging. The 3D imaging architectures presented in Ch. 4 each have their limitations and there is significant scope for future advances.

T-ray holography provides high speed 3D imaging of point scatterers in a homogenous background. The existing reconstruction algorithms may find application in identifying manufacturing defects or breast cancer screening (at longer wavelengths), however improved reconstruction algorithms are required for more general targets.

Similarly, the reconstruction algorithms employed in T-ray diffraction tomography impose relatively severe restrictions on the class of targets that may be imaged. There is a large body of research regarding the inversion of the wave equation for tomographic reconstruction in ultrasound and microwave fields without resorting to the first order approximations. Variations of these algorithms may prove fruitful in future T-ray DT systems. The Contrast Source Inversion algorithm is a notable candidate (van den Berg and Kleinman 1997).

The demonstrated T-ray DT system is only suitable for targets smaller than the THz sensor, which has a diameter of 2 cm. Future systems may utilise a telescope arrangement of THz polyethylene lenses to allow larger targets to be imaged. A further difficulty of T-ray DT is the low SNR caused by spreading the limited THz power (approximately 4 μ W average power) over the entire sensor area. T-ray DT systems will benefit greatly from higher power THz sources as they are developed. Future work may focus on extending T-ray DT to a reflection-mode architecture suitable for imaging a complementary class of targets.

6.3 Future Directions

T-ray CT is very attractive due to its ability to extract the frequency dependent refractive index at each pixel of a 3D image. The focused THz beam allows a higher SNR to be achieved than either of the other techniques. However, this technique is very time consuming due to the requirement to raster scan the target.

The T-ray CT reconstruction algorithm imposes a number of restrictions on the target. The extension of the system to more general targets represents an open problem of some significance.

Currently all 3D THz imaging techniques are hindered by low SNRs leading to reconstruction artifacts. This is especially problematic in frequency dependent reconstructions where accurate refractive index reconstruction is vital for spectroscopic identification applications. Accordingly, current spectroscopic applications are limited to 1D and 2D THz systems. THz tomography systems will benefit greatly from improved THz sources and detectors and it is anticipated that the frequency dependent information will yield important functional information and enable 3D material classification.

This Thesis has focused on femtosecond laser-based THz systems. However, the 3D imaging techniques that have been developed are portable to other THz systems – in particular, the implementation of these techniques with a high-power THz platform, using a synchrotron or free election laser, is an exciting future prospect that will enable imaging of a wide range of structures. This will perhaps create a new paradigm and allow THz science to delve into currently inaccessible realms.

Material Identification

Common THz systems employ averaging to improve the SNR, and deconvolution to remove systematic errors from the data. Each of these techniques have disadvantages and advanced signal processing methods have much to offer. Wavelet denoising has been shown to be highly effective. Future work in the wavelet domain will focus on using the wavelet transformed THz data for information processing and classification. Galvão et al. (2003) and Handley et al. (2004) have shown that the wavelet transform has promise as a method of feature extraction for material classification. Other applications include data compression (Handley et al. 2002) and refractive index estimation (Handley et al. 2001).

The most successful feature extraction techniques are often those derived from underlying knowledge of the system. As greater understanding of the interaction of THz radiation with different materials is obtained, this understanding may lead to improved

feature extraction algorithms. For instance, performing spectroscopic analysis of cryogenically cooled materials leads to insight into the fundamental molecular structure as higher order resonant modes are no longer populated. This in turn allows resonant frequencies to be identified for feature extraction.

There are a multitude of alternative classification algorithms. A thorough investigation of the available techniques was beyond the scope of this Thesis. However, recent progress in techniques such as Support Vector Machines may prove beneficial to future THz inspection systems.

The case studies conducted in Ch. 5 raise a large number of open questions. The powder spectroscopy study demonstrated that Rayleigh scattering is a critical concern in THz propagation through powdered substances. Current research is focused on attaining a greater understanding of THz scattering effects (Pearce and Mittleman 2001, Jian et al. 2003). The classification of materials independent of density, particle size and thickness is a difficult problem and would benefit from advanced models of THz propagation in random media.

Non-invasive cancer detection is a problem of paramount importance. The preliminary results in Ch. 5 show that THz spectroscopy can potentially be used to differentiate between cell cultures *in vitro*. One potential explanation for the detectable difference between the cells is the different production of extracellular matrix by the two cell types considered. Future controlled studies are required to verify these results and investigate its implications. The case study presents a simple experimental procedure for performing such experiments.

6.4 Summary of Original Contributions

The original contributions represented by this work are discussed in Sec. 1.5. In summary they include:

1. Improvement of 2D CCD based THz imaging systems. The techniques of synchronised dynamic subtraction and sensor calibration were developed and demonstrated.
2. T-ray holography. In collaboration with Shaohong Wang, the 2D time reversal THz imaging techniques of Ruffin et al. (2001) were extended to allow near real

- time 3D imaging of point scatterers. A reconstruction algorithm, based on the windowed Fourier transform was developed.
3. T-ray diffraction tomography. The principles of diffraction tomography, based on the Born and Rytov approximations to the wave equation, were applied to the THz regime for the first time. A practical 3D THz imaging system was demonstrated and diffraction tomography algorithms were used to reconstruct various targets. The limits of applicability of the Born and Rytov approximations were investigated experimentally.
 4. T-ray computed tomography. A high resolution, 3D, spectroscopic THz imaging system was developed, demonstrated and patented. In collaboration in Shao-hong Wang, an approximation to the Helmholtz equation was derived to allow linear reconstructions algorithms to be applied. The filtered backprojection algorithm was used to demonstrate frequency-dependent reconstruction of 3D targets with high fidelity.
 5. Phase estimation techniques. To improve the fidelity of T-ray CT reconstructions it was necessary to estimate the phase of THz pulses with high accuracy. Two techniques were developed to allow this to be performed: interpolated cross-correlation in the time-domain, and extrapolated phase unwrapping in the frequency-domain.
 6. THz spectroscopy classification framework. A set of algorithms were proposed and demonstrated to allow highly accurate classification of materials based on THz imaging data. Wavelet denoising was shown to significantly outperform Fourier methods when applied to pulsed THz data. Two feature extraction algorithms were developed. The first was based on linear filter coefficients, the second on deconvolved frequency coefficients. A genetic algorithm was developed to optimise the generalisation performance of a classifier.
 7. Case studies. Finally, several case studies were performed investigating the potential of THz imaging and material identification in a series of application areas. The power of the classification framework was demonstrated as highly accurate classification results were achieved. The case studies incorporated the first ever demonstrations of THz-TDS-based imaging of *Bacillus thuringiensis* and *in vitro* cultured cells.

6.5 In Closing

With every technological advance that has opened up new areas of the electromagnetic spectrum, there has been born a wealth of industries to apply that technology for the advancement of mankind – such is the promise of the THz regime (Abbott 2000). Modern THz imaging systems are in their infancy and are severely limited in comparison to the technology in neighbouring frequency bands. However, THz science continues to advance. This Thesis has contributed to this progress by developing imaging architectures and processing algorithms to extend THz imaging capabilities to new application domains. Toward the goal of three-dimensional THz inspection systems this Thesis presents significant and novel research on two parallel fronts. The first concerns 3D imaging architectures. Existing THz imaging systems were improved and adapted to design and test three different 3D tomography architectures complete with high-fidelity reconstruction algorithms. On the second front, a classification framework was designed to process THz spectroscopic images to allow specific materials to be identified. The classification framework was demonstrated in three case studies focusing on tissue identification, bacterial spore detection and cancer screening. These represent just three of the myriad of potential applications of this developing technology.

Appendix A

Hardware Specifications

This Appendix provides further detail and specifications on the components of the THz imaging systems utilised in this Thesis. It provides a list of the major hardware components along with their critical specifications and purpose.

Ultrafast laser. A Spectra-Physics Mai-Tai Ti:sapphire oscillator was used with a Hurricane regenerative amplifier. The specifications of this laser system include: 0.7 W output power at 802.3 nm, with a 1 kHz pulse repetition rate and 130 fs pulsewidth. The laser is used to produce the optical pump and probe beams used to generate and detect THz pulses.

Optical table. All of the THz imaging systems described in this Thesis were mounted on pneumatic vibration isolated optical tables. The tables were manufactured by Newport and had mounting holes, separated by 2.54 cm (1"), for optical posts.

Lock-in amplifier. A Stanford Research Systems SRS830 lock-in amplifier was used to digitise the detected optical signal and to perform phase sensitive filtering to improve the SNR. The lock-in amplifier was synchronised with an optical chopper.

Optical chopper. A Stanford Research Systems SR540 optical chopper was placed in the pump beam path and amplitude modulated the optical signal by means of a spinning slotted disk. The chopper controller provided manual control of the chopping frequency and provided a sync output which was connected to the lock-in amplifier. It also provided a sync input, which was driven when using synchronised dynamic subtraction.

Optical mirrors. The mirrors used for the NIR pump and probe beams were broadband metallic mirrors. These mirrors were Newport 10D20ER.2 or similar mirrors from other manufacturers.

Parabolic mirrors. Gold coated off-axis parabolic mirrors were used to focus and collimate the THz beam.

Linear motion stages. Three motorised motion stages were required for scanned THz imaging (two for raster scanning the target and a third for the optical delay line). A Newport MM3000 motion controller was used to control the three stages. This controller provided front panel control of the stages and GPIB control for remote access from a controller. The stages were Newport stepper motor UR73PP stages. They provided 200 mm of travel with a resolution of 1 μm .

Rotation stage. To rotate the imaging target, it was mounted on a motorised rotation stage. The stage was a NEMA23ESM stepper motor from Mil-Shaf Technologies. The motor was controlled using an A200SMC stepper motor controller from Mil-Shaf Technologies, which connected to the parallel port of a computer. The motor provided 1.8° resolution and a maximum speed of 120 revolutions per minute.

ZnTe crystals. Double side polished, $\langle 110 \rangle$ oriented ZnTe crystals were used for generation of THz pulses via OR and detection using EO sampling. For 2D FSEOS THz imaging a large 20 mm diameter crystal was used. A number of crystals were used in this Thesis. The crystal thickness varied between 3 mm and 4 mm. The crystals were purchased from eV Products.

GaAs wafers. Double side polished, high-resistivity GaAs wafers were used to construct photoconductive planar striplines by gluing two metal electrodes onto the wafer surface using conductive glue. A 0.6 mm thick, 3 cm diameter GaAs wafer was used with metal electrodes separated by 2 cm. High resistivity GaAs is available from a number of sources including University Wafer Pty. Ltd.

Quarter and half wave plates. Wave plates were used to rotate the polarisation of the NIR beam prior to splitting and photodetection. Broadband wave plates were required such as Newport 10RF42-3.

Polarising beam splitter. A cubic polarising beamsplitter was used to split the NIR laser pulses into pump and probe beams. The beamsplitter was anti-reflection coated for 800 nm and its part number was Melles Griot 03 PTA 101.

Spectrometer. A SPEX 500M spectrometer was used to disperse the wavelength components of the chirped optical probe pulse for the chirped probe imaging system described in Sec. 3.3.3. This spectrometer has a spectral resolution of 0.2 Å and a dispersion of 3 mm/nm.

Diffraction grating. A grating pair was used to chirp the optical probe pulse and extend its pulse width. The grating pair (grating constant $10\text{ }\mu\text{m}$) was setup so that the grating separation was 4 mm and the angle of incidence was 51° .

CCD Camera. A CCD camera was used in the 2D FSEOS THz imaging system and in the chirped probe system. The CCD used was a Princeton Instruments EEV576 $\times$ 384 CCD camera. It was air-cooled to -30° . The CCD pixel size was $22 \times 22\text{ }\mu\text{m}^2$. It provided 12 bit digitisation and a frame-transfer period of 15 ms. The CCD provided a sync output signal and allowed external triggering. It was controlled using the serial port of a computer.

Other optical components. A wide array of standard optical components were used in the experiments described in this Thesis. These include optical mounts and posts for attaching components to the optical table, iris diaphragms and IR viewers for aiding alignment, polarisers and photodiodes.

Appendix B

Software Implementation

A substantial amount of software was developed to support this research. Software tools were designed to control the equipment during an experiment and to process the results. This Appendix describes the major software applications used. It is impractical to provide full software listings of all software tools in this Appendix. Parties seeking further information should contact the author.

B.1 MFCPentaMax

This application (written in Microsoft Visual C++) was originally developed by Paul Campbell at Rensselaer Polytechnic Institute. It was used to control the PI Pentamax CCD camera and the motorised motion stages during 2D FSEOS THz imaging. The software was updated to allow it perform synchronised dynamic subtraction and to control the A200SMC stepper motor controller to allow it to be used for tomography experiments. The software set up the CCD camera and continuously streamed frames from the CCD to a memory buffer while the motion stages were programmed to move.

The software supported CCD pixel binning and dynamic subtraction and accumulation operations. The image data was saved to a file for offline processing and reconstruction which was performed using Matlab software (see Sec. B.4). A screenshot of the MFCPentaMax application is shown in Fig. B.1.

The code was compiled using Microsoft Visual Studio version 6.

B.2 Labview Tomography Application

National Instruments Labview was used to write general purpose experiment control programs due to the ease of programming and the wide support for equipment

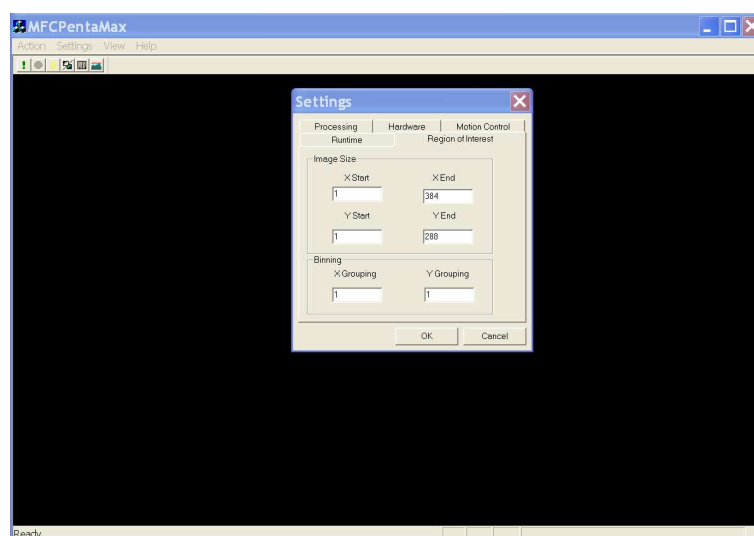


Figure B.1. Screenshot of the MFCPentamax software. This program was used to control 2D FSEOS THz imaging and tomography experiments. The program records images from the PI Pentamax CCD camera and controls the motorised motion stages to translate and rotate the target. The screenshot shows the CCD options setup page.

drivers. Existing programs written by members of the Department of Physics at Rensselaer Polytechnic Institute were modified to provide the desired functionality. Figure B.2 shows a screenshot of a Labview program designed for performing a T-ray CT experiment. The program allows three translation stages and a rotation stage to be controlled and reads the THz amplitude from a lock-in amplifier. The program plots the time-domain THz waveform and the 2D THz image in the windows shown. The result file is saved to disk for offline processing and reconstruction, which was performed using Matlab software (see Sec. B.4).

The Labview code was written in National Instruments Labview version 6i.

B.3 Slicer Dicer

The 3rd party software package Pixotec Slicer Dicer version 3.0.4 was used to generate the 3D surface rendered images presented in Ch. 4.

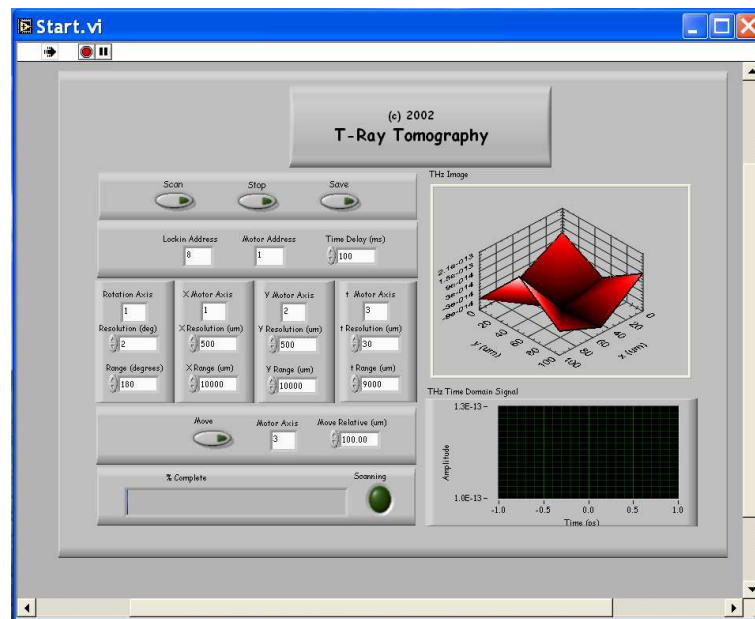


Figure B.2. Screenshot of the Labview tomography application. This program was developed to control T-ray CT experiments. The program allows three translation stages and a rotation stage to be controlled. The motion stages are controlled over a GPIB interface and the rotation stage is accessed through the parallel port. A lock-in amplifier is used to record the THz signal and is accessed over GPIB. The results of the experiment are plotted in the windows shown and may be saved to disk.

B.4 Matlab Code

Matlab 6.1 was used to implement all the algorithms described in this Thesis. Matlab is an interpreted programming language with built in support for a large number of mathematical functions and data presentation. Mathematical derivations were checked using the symbolic Maple toolbox. The following Matlab toolboxes were utilised:

- the wavelet toolbox,
- the system identification toolbox,
- the neural network toolbox,
- the symbolic toolbox,
- the signal processing toolbox, and
- the image processing toolbox.

B.4.1 Code Listings

The following sections provide code listings for the Matlab software used to implement many of the algorithms described in this Thesis. This is only a subset of the software developed to support this research. Matlab scripts with little algorithmic content, including those used to parse input data files and generate plots, have not been included. For more details on the software implementation please contact the author.

The attached CD includes copies of the Matlab files described below:

T-ray Holography –

holography2D.m This function implements the T-ray holography algorithms, as presented in Sec. 4.4. It demonstrates time domain Fresnel-Kirchoff back-propagation.

holography2Df.m This function extends the holography algorithms to operate in the frequency domain as required for 3D holography.

T-ray Computed Tomography –

reconCT.m This function presents the algorithms used for the reconstruction of T-ray CT targets as described in Sec. 4.6.

timingCT.m A subfunction used by reconCT. It implements the interpolated cross-correlation technique to estimate pulse timing.

thzCT2D.m Presents the algorithms used to process the high resolution 2D T-ray CT data.

T-ray Diffraction Tomography –

processDT.m A function used to perform sensor calibration for the T-ray DT data prior to reconstruction.

back.m The top level file for the T-ray DT reconstruction algorithm. It implements the algorithms described in Sec. 4.5.

findKappa.m A subfunction called by back.m.

findRay.m A subfunction called by back.m to implement spatial interpolation.

getDPhi.m A subfunction called by back.m to read in the DT data and filter it.

hammingImage.m A subfunction called by back.m to apply a 2D hamming window to the data.

interpolateDiffraction.m A subfunction called by back.m to apply the Fourier Diffraction Theorem and interpolate the result.

modulateImage.m A subfunction called by back.m.

Rytov.m A subfunction called by back.m to estimate the complex phase of the scattered field by the Rytov approximation.

Classification –

classificationTesting.m Presents a number of the classification schemes that are described in Ch. 5.

performClassification.m A subfunction called by classificationTesting.m.

pcaClassification.m This function implements Karhunen Loève based classification.

calcConfusionMatrix.m A subfunction called by classificationTesting.m to calculate the confusion matrix based on the classification results.

THz Pre-processing –

myUnwrap.m This function implements interpolated phase unwrapping in the frequency domain.

deconvolve.m This function deconvolves a THz pulse using a reference.

Refractive Index Estimation –

nNelderMead The top level function used to implement an iterative scheme to estimate the frequency dependent refractive index of a material. It is based on the method described in Appendix C.

simComp.m A subfunction called by nNelderMead.m.

fp_T_meas.m A subfunction called by nNelderMead.m.

calcHolderCorrection.m A subfunction called by nNelderMead.m. It is used when the THz sample is mounted in a holder or on a substrate.

duvill96Error.m A subfunction called by nNelderMead.m. It is used to calculate the error function for optimisation.

B.4 Matlab Code

T-ray Holography Functions

```
function [recon] = holography2D(theData,timeStep,range)
% HOLOGRAPHY2D Performs Fresnel–Kirchhoff backpropagation to reconstruct the target
%
% [recon] = holography2D(theData,timeStep,range)
%
% 'theData' contains a 3D array of THz diffraction data with respect to
% time, x and y. This data was measured using 2D FSEOS.
% The Fresnel–Kirchhoff diffraction equation is used to process the
% diffracted data to reconstruct the scattering target. 'range' specifies
% the distance to the target plane.
%
% Bradley Ferguson
% The University of Adelaide
% February 2002

% filter the data to remove the high frequency noise
figure(gcf+1);clf;
subplot(2,1,1)
imagesc(reshape(theData,200,[]));
theFiltData = medfilt2(reshape(theData,200,[]),[5,1]);
subplot(2,1,2);
imagesc(reshape(theFiltData,200,[]));

% consider a single point on the reconstructed plane at a time
P1x = 1; P1y = 1; % the position on the reconstruction plane
% (ie at the object)
t1 = -range; % (samples) the time at the object plane
r0 = 30e-3; % (m) the perpendicular distance between the two planes
resXY = 20e-3/ size(theData,2); % (m) the size of each pixel
resTime = timeStep; % (s) the delay of each sample
c = 3e8; % (m.s-1) the speed of light.
tRange = 100;

% we will need to have the derivative of the measured data
dttheData = diff(theData);
dttheFiltData = diff(theFiltData);
figure(gcf+1);clf;
subplot(2,1,1);
imagesc(dttheData);
subplot(2,1,2);
imagesc(dttheFiltData);

dttheData = dttheFiltData;

UP1 = zeros(size(theData,2),size(theData,3),tRange+1);

for t1Index = 1:tRange
    t1 = -range -tRange/2 + t1Index;

    for P1x = 1:size(theData,3)
        for P1y = 1:size(theData,2)
```



```

xIndex = [1:size(theData,3)];
P0XIndex = repmat(xIndex, size(theData,2),1);

yIndex = [1:size(theData,2)]';
P0YIndex = repmat(yIndex,1, size(theData,3));

% calculate the distance from the object point to every point
% on the image plane
r01 = sqrt(r0^2+(((P0XIndex - P1x)*resXY).^2 + ((P0YIndex - ...
    P1y)*resXY).^2));

% calculate the zenith angle between the two points.
cosTheta = r0./r01;

% calculate the time at the image plane
t0 = round(t1+r01/c/resTime); % (samples)

% find the pixels at which the time is out of range.
overRange = find(t0>size(dttheData,1));
underRange = find(t0<1);

t0(overRange) = 1;
t0(underRange) = 1;

% make an array consisting of the indexes into the ddt matrix
t0Index = sub2ind(size(dttheData), reshape(t0,1,[]), reshape(P0YIndex,1,[]), ...
    reshape(P0XIndex,1,[]));

ddt = dttheData(t0Index)';

ddt(overRange) = 0;
ddt(underRange) = 0;

intExp = cosTheta/2/pi/c./r01.*ddt;
UP1(P1y,P1x,t1Index) = -sum(sum(intExp));

end

end

end

figure(gcf+1);clf;
x = reshape(UP1, size(theData,2),[]);
xAxis = [-size(x,2)/2:size(x,2)/2-1] * resTime * 1e12;
yAxis = [-size(x,1)/2:size(x,1)/2-1] * resXY * 1e3;
imagesc(xAxis,yAxis,x);
formatImage(3); grid off;
xlabel('Time (ps)');
ylabel('Width (mm)');

if (printPlots == 1)
    print(printOpts, strcat(printPath, 'THzFieldImage'));

```

B.4 Matlab Code

```
end
```

```
figure(gcf+1);clf;
plot(yAxis,UP1(:,1),size(UP1,3)/2)*1e6);
formatImage(3);
xlabel('Width (mm)');
ylabel('THz Intensity (a.u.)');

if (printPlots == 1)
    print(printOpts, strcat(printPath, 'THzFieldDist'));
end
```

```
function [range] = holography2DF(theDataF,freq,freqStep)
% HOLOGRAPHY2DF Performs Fresnel–Kirchhoff backpropagation to reconstruct the
% target in the frequency domain
%
% [recon] = holography2D(theDataF,freq,freqStep)
%
% 'theDataF' contains a 3D array of THz diffraction data with respect to
% freq, x and y. This data was measured using 2D FSEOS.
% The Fresnel–Kirchhoff diffraction equation is used to process the
% diffracted data to reconstruct the scattering target.
% The reconstruction is iteratively performed at multiple ranges
% to determine the distance to the target plane.
%
% The algorithm performs the reconstruction at multiple ranges and returns
% the distance at which the reconstructed field is maximised.
%
% Bradley Ferguson
% The University of Adelaide
% February 2002

fI = floor(freq*1e12/freqStep);
xyfSlice = theDataF(fI,:,:)
xyfSlice = shiftdim(xyfSlice,1); xyfSlice = xyfSlice / max(max(xyfSlice));
xyfSlice = wiener2(xyfSlice,[2,2]);

% use the symmetry to reduce our work load
theData = mean(xyfSlice,2);

i=1; clear totalUP;
allDists = [44e-3:0.25e-3:50e-3];
for r0 = 44e-3:0.25e-3:50e-3 % (m) the perpendicular distance between
                             % the two planes

    % consider a single point on the reconstructed plane at a time
    P1x = 1; P1y = 1; % the position on the reconstruction plane
                       % (ie at the object)
    resXY = size(theData,2); % (m) the size of each pixel
    resTime = timeStep; % (s) the delay of each sample
    c = 3e8; % (m.s-1) the speed of light.
```

```

lambda = c/freq/1e12;
k = 2*pi/lambda;

UP1 = zeros(size(theData,1),size(theData,2));

for P1x = 1:size(theData,2)
    for P1y = 1:size(theData,1)

        xIndex = [1:size(theData,2)];
        P0XIndex = repmat(xIndex,size(theData,1),1);

        yIndex = [1:size(theData,1)]';
        P0YIndex = repmat(yIndex,1,size(theData,2));

        % calculate the distance from the object point to every point
        % on the image plane
        r01 = sqrt(r0^2+(((P0XIndex - P1x)*resXY).^2 + ...
            ((P0YIndex - P1y)*resXY).^2));

        % calculate the zenith angle between the two points.
        cosTheta = r0./r01;

        % calculate the phase term to apply
        phaseTerm = exp(-j*k*r01);

        intExp = cosTheta./lambda./r01.*phaseTerm;
        UP1(P1y,P1x) = sum(sum(intExp));

    end
    fprintf('%i ',P1x);
end

totalUP(:,i) = UP1;
i=i+1

end

[a,dist]=max(abs(totalUP));
range = allDists(dist);

```

T-ray CT Functions

```

function [reconCT,sinogramOut] = reconCT(sinogram,minThreshSinogram,filtSinogram,...
    reconLowThresh,reconHighThresh,dX,dAngle,debugPlot)
% RECONCT Computes the inverse radon transform for the slice of data.
%
% [reconCT,finalSinogram] = reconCT(sinogram,minThreshSinogram,filtSinogram,...
%     reconLowThresh,reconHighThresh,dX,dAngle,debugPlot)
%
% This function calculates the iradon function after applying some pre and post

```

B.4 Matlab Code

```
% processing on the data.
%
%
% Bradley Ferguson
% The University of Adelaide
% February 2003
%

if (nargin < 2)
    minThreshSinogram = 0;
end

if (nargin < 3)
    filtSinogram = 0;
end

reconThresh = 1;
if (nargin < 5)
    reconThresh = 0;
end

if (nargin < 8)
    debugPlot = 0;
end

sinogramOut = sinogram;

% preprocess the sinogram
if (minThreshSinogram ~= 0)
    sinogramOut = sinogram - min(min(sinogram));
    sinogramOut(sinogramOut < minThreshSinogram) = 0;
end

if (filtSinogram == 1)
    % wrap around the top and bottom rows of the delay and Wiener filter
    wrapSinogram = [sinogramOut(end,:); sinogramOut; sinogramOut(1,:)];
    filtSinogram = wiener2(wrapSinogram,[2,2]);
    sinogramOut = filtSinogram(2:end-1,:);
end

if (debugPlot == 1)
    figure(gcf+1); clf;
    imagesc([0:size(sinogramOut,2)-1]*dX,[0:size(sinogramOut,1)-1]*dAngle,sinogramOut);
    formatImage(2);
    title('Sinogram');
    ylabel('Angle (degrees)');
    xlabel('X (mm)');
end

reconCT = iradon(sinogramOut',[], 'spline', 'hamming', 100);

if (reconThresh == 1)
    reconCT = normMatrix(reconCT);
```

```

    reconCT = threshMatrix(reconCT, reconLowThresh, reconHighThresh, 1);
end

if (debugPlot == 1)
    figure(gcf+1); clf;
    imagesc([0:size(reconCT,1)]*dX,[0:size(reconCT,2)]*dX,reconCT);
    formatImage(2);
    title('Reconstruction');
    ylabel('Y (mm)');
    xlabel('X (mm)');
end



---



function [reconCT, sinogram] = timingCT(theSlice, refPulse, stepAngle, debugPlot)
% TIMINGCT Computes the inverse radon transform for the slice of data files using the
%           interpolated cross-correlation method to estimate phase.
%
% [reconCT, sinogram] = timingCT(theSlice, refPulse, stepAngle, debugPlot)
%
% This function used interpolated cross-correlation to generate
% a timing sinogram for the 2D THz CT data in 'theSlice'.
% The reference THz waveform is provided in 'refPulse'.
% 'stepAngle' specifies the angular resolution of the measurements.
% The inverse Radon transform is used to reconstruct the sinogram data.
%
% Bradley Ferguson
% The University of Adelaide
% October 2001
%

nX = size(theSlice, 2);
nTheta = size(theSlice, 3);

interpVal = 1;
xcorrTiming = zeros(nX, nTheta);
ztheSlice = theSlice;
ztheSlice = ztheSlice - min(min(min(ztheSlice)));

theRange = [120:160];

if 1==0
    for x = 1:nX
        for theta = 1:nTheta
            [corrVal, corrIndex] = xcorr(interp(refPulse(theRange), interpVal), ...
                interp(ztheSlice(theRange, x, theta), interpVal));
            [corrMax, corrTiming] = max(corrVal);
            xcorrTiming(x, theta) = -1*corrIndex(corrTiming);
        end
    end
else
    for theta = 1:nTheta
        [corrVal] = xcorr2((refPulse(theRange)), (ztheSlice(theRange, :, theta)));
    end
end

```

B.4 Matlab Code

```
[corrMax,corrTiming] = max(corrVal,[],1);
xcorrTiming(:,theta) = -1*(corrTiming-length(theRange))';
end
end

xcorrTimingCT = iradon(xcorrTiming,stepAngle,65,'spline','Hamming');

% use the xcorr reconstruction.
%
xcorrTimingCTnn = xcorrTimingCT;
sinogram = xcorrTiming;
reconCT = xcorrTimingCTnn;

% now plot the sinograms for each of these.
if (debugPlot == 1)
    figure(gcf+1); clf;
    imagesc(xcorrTiming);
    formatImage;
    title('XCORR Timing');
    xlabel('angle (degrees)');
    ylabel('mm');

    figure(gcf+1); clf;
    imagesc(xcorrTimingCT);
    axis off;
    title('XCORR timing');
    formatImage;

    figure(gcf+1); clf;
    imagesc(xcorrTimingCTnn)
    figure(gcf+1); clf;
    imagesc(dilatedMap);
end
```

```
% Script: thzCT2D Calculates the 2D T-ray CT reconstruction
%
% This function opens the 2D THz files CT file and
% computes the inverse Radon Transform to obtain an image of
% the slice.
%
% Bradley Ferguson
% The University of Adelaide
% February 2003
%

figure(1); clf;
printPlots = 0;
printThesisPlots = 1;
printOpts = '-deps2c';

openFile = 1;
```

```

plotSinograms = 1;
crossCorr = 1;
reconstruct = 1;
freqDomain = 1;
refractiveIndex = 1;
reconAllPhases = 1;

% impose sensible limits on the data. This
% helps regularise the results.
delayMin = 6;
interpMin = 20;
phaseMin = 0.6;
delayReconMin = 0.58;
delayReconMax = 1;
interpReconMin = .35;
interpReconMax = .7;
phaseReconMin = 0;
phaseReconMax = 1;
printName = 'c:\users\bsf\documents\thesisfigs\process_030215_sample1_';

% open the file and read the header information
fid = fopen(fileName, 'r', 'n');
mHeader = fscanf(fid, '%f', 8); % 6, 'int32')

mDat = fscanf(fid, '%f');
fclose(fid);

nX = ceil(mHeader(1)/mHeader(2))+1;
dX = mHeader(2) / 1000; % mm
nY = ceil(mHeader(3)/mHeader(4))+1;
dY = mHeader(4) / 1000; % mm
nTime = ceil(mHeader(5)/mHeader(6))+1;
dTime = mHeader(6) / 1.5e8 * 1e6; % ps
time = [0:nTime-1]*dTime;

nAngle = ceil(mHeader(7)/mHeader(8));
dAngle = mHeader(8); % degrees

mDat = reshape(mDat, nAngle, nTime, nX*nY);

[amp, delay] = max(mDat(:, 1:1:end, :), [], 2);

amp = reshape(amp, nAngle, nX*nY);
delay = reshape(delay, nAngle, nX*nY);
end

if (crossCorr == 1)
    % use cross-correlation to get the delay.
    interpFactor = 10;
    subsampleTime = 2; % set to 2 to skip every second sample

    % first interpolate the signals to improve the resolution

```

B.4 Matlab Code

```
refInterp = interpft(mDat(2,1:subsampleTime:end),nTime*interpFactor);
interpDelay = zeros(nAngle,nX);
for i = 1:nAngle
    g = interpft(mDat(i,1:subsampleTime:end,:),nTime*interpFactor);

    % note xcorr2 is much slower than this loop
    for j = 1:nX*nY
        h = xcorr(g(:,j),refInterp);
        % h = abs(h);
        h = boxfilt(h,60);
        [a,b] = max(h);
        interpDelay(i,j) = b;
    end
end

% illustrate the phase estimation process
interpSingle = interpft(mDat(12,1:subsampleTime:end),nTime*interpFactor);
h = xcorr(interpSingle,refInterp);
interpTime = [1:nTime*interpFactor]*dTime/interpFactor;

figure(gcf+1);
clf;subplot(2,1,1);
time2 = time(1:2:end); m=max(mDat(12,1:subsampleTime:end),25));
plot(time2,mDat(12,1:subsampleTime:end),m,'b—x')
hold on
m=max(h); of = 12;
plot(interpTime,(h(ceil(nTime*interpFactor/2+of):ceil(nTime*interpFactor/2 ...
+of)+nTime*interpFactor-1))/m,'r')
formatImage(1);
xlabel('time (ps)')
ylabel('Amplitude (a.u.)');
legend('THz pulse','Interpolated cross correlation');

if (printThesisPlots)
    print(printOpts, strcat(printName,'xcorrInterpComp'));
end

figure(gcf+1);clf;
imagesc([0:nX*nY-1]*dY,[0:nAngle-1]*dAngle,interpDelay);
formatImage(2);
% title('XCorr Timing Sinogram');
ylabel('Angle (degrees)');
xlabel('Offset (nm)');

if (printThesisPlots)
    print(printOpts, strcat(printName,'xCorrSinogram'));
end

% compare xcorr and raw delay estimation
figure(gcf+1);clf;
subplot(2,2,1)
imagesc([0:nX*nY-1]*dY,[0:nAngle-1]*dAngle,interpDelay);
formatImage(1);
```



```

% title('XCorr Timing Sinogram');
ylabel('Angle (degrees)');
xlabel('Offset (mm)');
title('(a)');

subplot(2,2,2)
imagesc([0:nX*nY-1]*dY,[0:nAngle-1]*dAngle,delay);
formatImage(1);
% title('XCorr Timing Sinogram');
ylabel('Angle (degrees)');
xlabel('Offset (mm)');
title('(b)');
if (printThesisPlots)
    print(printOpts, strcat(printName, 'comparePhaseSinogram'));
end
end

if (freqDomain == 1)
    fftPad = 8; % interpolation factor for the FFT.
    timeSubsample = subsampleTime;

    fDat = fft(shiftDim(mDat(:,1:timeSubsample:end),1),nTime*fftPad/timeSubsample);

    freq = [0:nTime*fftPad/timeSubsample-1]/(dTime*timeSubsample)/...
        (fftPad*nTime/timeSubsample-1);
    dFreq = freq(2);

    testNormalUnwrapping = 1;
    if (testNormalUnwrapping == 1)
        fPhase = unwrap(angle(fDat));
        maxFreq = 3; % THz
        maxFreqIndex = ceil(maxFreq / freq(2));
        fPhaseNorm = fPhase;
    end

    fPhase = myUnwrap(fDat,dFreq,0.2,0.4);
    maxFreq = 3; % THz
    maxFreqIndex = min(ceil(size(fPhase,1)/2),ceil(maxFreq / freq(2)));

    % compare normal and extrapolated frequency domain phase unwrapping.
    maxFreq = 1.8; % THz
    maxFreqIndex = min(ceil(size(fPhase,1)/2),ceil(maxFreq / freq(2)));

    figure(gcf+1);clf;subplot(2,1,1)
    plot(freq(1:maxFreqIndex),fPhase(1:maxFreqIndex,ceil(2/3*size(fPhase,2))),...
        ceil(2/3*size(fPhase,3)),'b')
    hold on
    plot(freq(1:maxFreqIndex),fPhaseNorm(1:maxFreqIndex,ceil(2/3*size(fPhase,2))),...
        ceil(2/3*size(fPhase,3)),'r—')
    formatImage(1);
    xlabel('frequency (THz)');
    ylabel('phase (radians)');

```

B.4 Matlab Code

```
legend('extrapolated unwrapping','standard unwrapping');

if (printThesisPlots)
    print(printOpts, strcat(printName, 'PhaseUnwrapComp'));
end

% take the phase at a frequency of 1 THz.
THzFrequency = 1.0;
THzIndex = ceil(THzFrequency/freq(2));
phase1THz = reshape(fPhase(THzIndex, :, :), nX*nY, nAngle);
phase1THz = phase1THz';

figure(gcf+1); clf;
imagesc([0:nX*nY-1]*dY, [0:nAngle-1]*dAngle, phase1THz);
formatImage(1);
title('Fourier Phase (1 THz) Sinogram');
ylabel('Angle (degrees)');
xlabel('X (mm)');

if (printPlots)
    print(printOpts, strcat(printName, 'freqPhaseSinogram'));
end
end

if (plotSinograms == 1)
    imagesc([0:nX*nY-1]*dY, [0:nAngle-1]*dAngle, amp);
    formatImage(2);
    %title('Amplitude Sinogram');
    ylabel('Angle (degrees)');
    xlabel('Offset (mm)');

    if (printThesisPlots)
        print(printOpts, strcat(printName, 'ampSinogram'));
    end

    figure(gcf+1); clf;
    imagesc([0:nX*nY-1]*dY, [0:nAngle-1]*dAngle, delay);
    formatImage(2);
    % title('Phase Sinogram');
    ylabel('Angle (degrees)');
    xlabel('Offset (mm)');

    if (printThesisPlots)
        print(printOpts, strcat(printName, 'phaseSinogram'));
    end

    wrappedDelay = [delay; delay];
    imagesc([0:nX*nY-1]*dY, [0:2*(nAngle-1)]*dAngle, wrappedDelay);
    formatImage(2);
    title('Phase Sinogram (360 degrees)');
    ylabel('Angle (degrees)');
    xlabel('X (mm)');
```

```

    if (printPlots)
        print(printOpts, strcat(printName, '360phaseSinogram'));
    end
end

if (refractiveIndex == 1)
    [recon, sino]=reconCT(interpDelay,interpMin,1);
    reconN = recon *dTime/interpFactor/1e12/dY/1e-3 * 3e8;

    figure(gcf+1);clf;
    imagesc([0:size(reconN,1)-1]*dX,[0:size(reconN,2)-1]*dX, fliplr(flipud(1+reconN)));
    axis square; axis image;
    set(gca, 'XTick',[10:10:size(reconN,1)*dX]);
    set(gca, 'YTick',[10:10:size(reconN,1)*dX]);
    axis xy
    colorbar;
    formatImage(2);
    %title('Reconstructed Refractive Index');
    ylabel('z (mm)');
    xlabel('x (mm)');
    if (printThesisPlots)
        print(printOpts, strcat(printName, 'reconNxcorr'));
    end

    % produce 3D images.
    w = wiener2(reconN);
    g = surf([0:size(reconN,1)-1]*dX,[0:size(reconN,2)-1]*dX, fliplr(flipud((1+w))));
    set(gca, 'XTick',[10:10:size(reconN,1)*dX]);
    set(gca, 'YTick',[10:10:size(reconN,1)*dX]);
    axis xy; axis tight;
    g = findobj(gcf, 'fontsize',10);
    set(g, 'fontsize',13);
    set(gca, 'fontsize',13);

    xlabel('x (mm)');
    ylabel('z (mm)');
    zlabel('n');
    view(-37.5,76);
    if (printThesisPlots)
        print(printOpts, strcat(printName, 'recon3DN'));
    end

    [recon, sino]=reconCT(-phase1THz,phaseMin,1);
    reconN = recon / 2/pi / THzFrequency/1e12/dY/1e-3 * 3e8;
    figure(gcf+1);clf;
    imagesc([0:size(reconN,1)*dX,[0:size(reconN,2)]*dX,1+reconN);
    axis square; axis image;
    set(gca, 'XTick',[10:10:size(reconN,1)*dX]);
    set(gca, 'YTick',[10:10:size(reconN,1)*dX]);

```

B.4 Matlab Code

```
axis xy
colorbar;
formatImage(2);
title('Reconstructed Refractive Index');
ylabel('Y (mm)');
xlabel('X (mm)');
if (printPlots)
    print(printOpts, strcat(printName, 'reconNfreq'));
end

% produce 3D images.
w = wiener2(reconN);
figure(gcf+1); clf;
if (open_2_24 == 1)
    w = fliplr(w);
end

g = surf([0:size(reconN,1)-1]*dX,[0:size(reconN,2)-1]*dX, fliplr(flipud((w))));
set(gca, 'XTick', [10:10:size(reconN,1)*dX]);
set(gca, 'YTick', [10:10:size(reconN,1)*dX]);
axis xy; axis tight;
g = findobj(gcf, 'fontsize', 10);
set(g, 'fontsize', 13);
set(gca, 'fontsize', 13);

xlabel('X (mm)');
ylabel('Y (mm)');
zlabel('n');
view(-37.5,76);
if (printPlots)
    print(printOpts, strcat(printName, 'recon3DNfreq'));
end

end

if (reconstruct == 1)
    [recon, sino]=reconCT(delay, delayMin, 1, delayReconMin, delayReconMax, dY, dAngle, 1);
    if (printPlots)
        figure(gcf-1);
        print(printOpts, strcat(printName, 'peakTimingSinogram'));
        figure(gcf+1);
        print(printOpts, strcat(printName, 'peakTimingRecon'));
    end

    [recon, sino]=reconCT(interpDelay, interpMin, 1, interpReconMin, ...
        interpReconMax, dY, dAngle, 1);
    if (printPlots)
        figure(gcf-1);
        print(printOpts, strcat(printName, 'xcorrSinogram'));
        figure(gcf+1);
        print(printOpts, strcat(printName, 'xcorrRecon'));
    end
end
```

```

[recon , sino]=reconCT(-phase1THz,phaseMin,1,phaseReconMin,...
    phaseReconMax,dY,dAngle,1);
if (printPlots)
    figure(gcf-1);
    print(printOpts, strcat(printName, 'fourierPhaseSinogram'));
    figure(gcf+1);
    print(printOpts, strcat(printName, 'fourierPhaseRecon'));
end
end

```

T-ray DT Functions

```

function [processedDTSlice,freqAmp,freqPhase,actualFreq] = processDT(DTangleDat,...
    Ref,timeStep,frequency,method,debugPlotIn)
% processDT Processes the DT slice by subtracting the reference.
%
% [processedDTSlice] = processDT(DTangleDat,Ref,timeStep,frequency,method,...
%     debugPlotIn))
%
% A sensor calibration method is implemented and
% tested. This process subtracts the incident field to
% calculate the scattered field. It then normalises
% the scattered data to account for sensor non-linearity.
%
% Bradley Ferguson
% The University of Adelaide
% July 2002

if (nargin >= 6)
    debugPlot = debugPlotIn;
else
    debugPlot = 0;
end

% try first in the time domain....
% perform the following steps:
% 1. subtract the scaled ref in the time domain
% 2. normalise the data with the peaks of the ref pulses
%     (to remove sensor inhomogeneity.)
%
processedDTSlice = DTangleDat;

% 1. subtract the scaled ref in the time domain
processedDTSlice = processedDTSlice - Ref.*refScale;

% 2. normalise the data with the peaks of the ref pulses
%     (to remove sensor inhomogeneity.)
normRefPeaks = refPeaks / max(max(refPeaks));

```

B.4 Matlab Code

```
% for some values of the background this results in division by zero
% and v. large numbers in the normalized matrix.
normRefPeaks(normRefPeaks < 0.2) = 1;

normBackground = repmat(normRefPeaks,[size(DTangleDat,1),1,1]);
processedDTSlice = processedDTSlice ./ normBackground;

% 5. Fourier transform and save the frequency of interest.
fProcDT = fft(processedDTSlice,size(Ref,1)*2);

fStep = 1/timeStep/size(Ref,1)/2;
fIndex = round(frequency/fStep);

freqAmp = abs(fProcDT(fIndex,:,:));
freqPhaseAll = unwrap(angle(fProcDT(1:end/4,:,:)));
freqPhase = freqPhaseAll(fIndex,:,:);

actualFreq = fIndex * fStep;

if (debugPlot)
    x = 45; % floor(size(Ref,2)/2);
    y = 35; % floor(size(Ref,3)/2);

    theTime = [0:size(DTangleDat,1)-1]*timeStep * 1e12;
    figure(gcf+1);
    clf;
    plot(theTime,DTangleDat(:,x,y))
    hold on;
    plot(theTime,Ref(:,x,y),'r');
    plot(theTime,processedDTSlice(:,x,y),'g');
    formatImage(2);
    xlabel('time (ps)');
    legend('Diffracted','Reference','Processed');
end

% function [reconData] = back(fileNameIn,k,m,N,nd,h,i,d,l,w,r,b,phi0,s,t,l0)
% BACK Implements diffraction tomography algorithm.
%
% [reconData] = back ( fileNameIn,k,m,N,nd,h,i,d,l,w,r,b,phi0,s,t,l0)
%
% This function is the header function for the diffraction tomography
% software. This code is based on diffraction tomography code
% by Malcolm Slaney.
%
% Kak-A. C. and Slaney-M. (2001). Principles of Computerized
% Tomographic Imaging, Society of Industrial and Applied Mathematics
%
% o fileName – the name of the data file to open
% o k – the number of projections
% o m – the number of rays
% o N – the reconstruction grid size
```

```

%      o nd – the number of depths for filtered backpropagation
%      o h – perform Hamming window
%      o i – estimate object function
%      o d – double projection size
%      o l – low pass filter before IFFT
%      o w – use |w| filter in backpropagation
%      o r – use Rytov/Born approximation
%      o b – use backpropagation/interpolation
%      o s – reconstruction sampling interval (lambda)
%      o t – receiver sampling interval
%      o l0 – distance to receiver plane
%
%      Bradley Ferguson
%      The University of Adelaide
%      March 2001
%

% parse the input parameters
rytovf = r; doham = h; backf = b; objectFunction = o; tribolet = 0;
double = d; lowPass = l; omegaFilter = w; M = m; T = t; ifn = fileName;
K = k; nDepth = nd;
K0 = 2*pi;
DEBUG = 0;
BILINEAR = 1;
RYTOV_PHASE_FILES = 1;
N2 = N/2; K2 = K/2; M2 = M/2;

if (DEBUG)
    figure(1); clf;
end

% find the log (base 2) of M and N;
logM = 0;
while(bitshift(1,logM)<M)
    logM = logM + 1;
end

logN = 0;
while(bitshift(1,logN)<N)
    logN = logN + 1;
end

% note I don't do any error checking on the input parameters.
% I may add this later.

if (double)
    M = 2*M;
    M2 = M/2;
    M4 = M/4;
    logM = logM + 1;
end

if (backf)

```

B.4 Matlab Code

```
        PropagateDiffraction;
else
        InterpolateDiffraction;
end

% perform some checks
realenergy = sum(sum(real(Object).^2));
imenergy = sum(sum(imag(Object).^2));

fprintf('Recon quality is %f\n',realenergy/imenergy);

% calculate the refractive index if required.
% O = (1+ndelta)^2 - 1
% therefore
% ndelta = +\ - sqrt(O+1) - 1
% we choose the root that is closest to +1

if (~objectFunction)
    Object = sqrt(Object+1);
    % TBD invert if negative.
    Object = Object - 1;
end

% create the output picture
pic = abs(Object);
```

```
function [kappa] = findKappa(j,M,T)
% FINDKAPPA - Map the index of a fft
%           into the proper frequency in the
%           receiver plane (kappa)
%           * j - Index of Ray
%           * M - Number of points in projection
%           * T - Sampling interval
%
%   Bradley Ferguson
%   The University of Adelaide
%   March 2002
%
kappa = (2.0*pi/(M)/(T)*((j)-M/2))
```

```
function [k,l,alpha,beta,rotation] = findray(u,v,solution,M,K,T)
% FINDRAY - Determine the projection and ray number corresponding to point.
%
% [k,l,alpha,beta,rotation] = function findray(u,v,solution,M,K)
%   Given a point in two dimensions this routine finds the projection and ray
%   number that provide data about the desired point
%
%   Inputs
```

```
% The u and v coordinates of the point that is to be estimated
% from the available data. These numbers should be normalized by
% K0. The max should be 2, with the circle of radius K0
% appearing at radius of 1.
% The solution number desired (0 or 1)
% The number of rays and projections (M and K).
%
% Outputs
% This routine returns integers k and l representing the ray and
% projection numbers. It also returns alpha and beta which are the
% points in the diffraction space (see Devaney for this coordinate
% system).
%
% Bradley Ferguson
% The University of Adelaide
% March 2002.
%
```

```
M2 = M/2; K2 = K/2;
```

```
% we only do Mueller mode.
```

```
r = sqrt(u^2+v^2);
```

```
theta = atan2(v,u);
```

```
if (r^2 <=2)
```

```
    beta = 2 * asin(r/2); % calculate ray angle
```

```
    if (solution == 0)
```

```
        alpha = theta + beta/2 + pi/2;
```

```
    else
```

```
        beta = -beta;
```

```
        alpha = theta + beta/2 + 3*pi/2;
```

```
    end
```

```
    if (alpha < 0)
```

```
        alpha = alpha + 2*pi;
```

```
    end
```

```
    alpha=alpha/2/pi*K;
```

```
    beta = M*T*sin(beta)+M2;
```

```
else
```

```
    % fprintf('Illegal bounds for u and v in <findRay>\n');
```

```
    alpha = -1; beta = -1;
```

```
end
```

```
k = alpha + 0.5;
```

```
l = beta;
```

```
rotation = alpha;
```

```
% GETDPHI Read projection data and filter it.
```

```
%
```

```
% The output of this script is D_phi_0 as in equation (28) of
```

```
% Devaney A., 'A filtered backpropagation algorithm for diffraction
```

B.4 Matlab Code

```
% tomography.' It is the estimate of the object's Fourier
% transform along circular arcs.
%
% Bradley Ferguson
% The University of Adelaide
% March 2001
%

% build a Hamming window (if required)
if (double)
    getDPhi_window = zeros(M,1);

    if (doham)
        getDPhi_window(M4+1:M4+M2) = hamming(M2);
    else
        getDPhi_window(M4+1:M4+M2) = ones(M2,1);
    end
else
    if (doham)
        getDPhi_window = hamming(M);
    else
        getDPhi_window = ones(M,1);
    end
end

% now invert every second value of the window
getDPhi_window(1:2:end) = -1*getDPhi_window(1:2:end);

% replicate the window for each projection angle
getDPhi_window = repmat(getDPhi_window,1,K);

if (DEBUG)
    figure(gcf+1); clf;
    imagesc(getDPhi_window);
    title('Hamming window to filter input data');
end

% now open the file... (note: it contains complex values).

ifp = fopen(ifn,'r','n');
if (ifp == -1)
    fprintf('Error opening file in <getDPhi>\n');
    return;
end

[tempField,count] = fread(ifp,'float32');
fclose(ifp);

Field = tempField(1:2:end-1) + j*tempField(2:2:end);

% reshape the field
if (~double)
```

```

    Field = reshape(Field,M,K);
else
    size(Field)
    M2
    K
    Field = reshape(Field,M2,K);

    % we need to pad the data with zeros...
    dField = zeros(M,K);
    dField(M4+1:M2+M4,:) = Field;
    Field = dField; clear dField;
end

if (DEBUG)
    figure(gcf+1); clf;
    imagesc(abs(Field));
    title('Input Field');
end

if (rytovf)
    Rytov;
end

% multiply each projection by the window.
Field = Field .* getDPhi_window;

% take the Fourier transform of the windowed field
Field = fft(Field);

% now undo the effect of inverting every second window element
Field(1:2:end,:) = -1* Field(1:2:end,:);

if (DEBUG)
    figure(gcf+1); clf;
    imagesc(log10(abs(Field)));
    title('FFT of input field (db)');
end

% now multiply each term by :
%
%       $-2i \cdot \gamma \cdot \exp(-i \cdot \gamma \cdot 10) / K^2$ 
%
% we also multiply by 't' to account for the sampling interval in the integral.
% this gives a valid estimate of the FT of the field.
%
% note:  $\kappa = 2\pi / M T \cdot (j - M/2)$  where j is the index of the projection.
%       $\kappa$  is the one dimensional frequency of the scattered field along the
%      receiver line.
% note:  $\gamma = \sqrt{k_0^2 - \kappa^2}$ 

kappa = (([0:M-1] - M/2)*2*pi/M/T)';
gammaSquared = K0^2 - kappa.^2;

```

B.4 Matlab Code

```
gammaSquared(find(gammaSquared < 0)) = 0;
gamma = sqrt(gammaSquared);

scale = j*2*T*gamma/K0^2.*exp(-j*gamma*10);

% repeat the scale matrix for each projection
scale = repmat(scale,1,K);

% scale the field
Field = Field .* scale;

if (DEBUG)
    figure(gcf+1);clf;
    imagesc(log10(abs(Field)));
    title('FFT of Scattered Field');
end
```

```
function [hammingImage] = hammingImage(pic,size,center)
% CHAMMING
%
%      Multiply the Fourier transform of an image
%      by a two dimensional Hamming window.  There are
%      three parameters...the address of the picture,
%      its size and a single flag indicating where the
%      center (origin) of the picture is...center = 0
%      implies that the center of the picture is in
%      the upper left hand corner...i.e. the normal
%      fft position.  Anything else tells this routine that
%      the array has its center in the center of the
%      array.
%
%      Bradley Ferguson
%      The University of Adelaide
%      March 2002.
%

    f = 2*pi/(size-1);
    N = [0:size-1];

    N2 = size/2;

    if (center)
        % /* Pic Origin at center */
        w = 0.54 + 0.46*cos(f*(N-N2));
    else
        % /* Pic origin at upper LH corner */
        w = 0.54 + 0.46*cos(f*(N));
    end

    hammingMap = repmat(w,size,1).*repmat(w',1,size);
    hammingImage = pic .* hammingMap;
```

```

% InterpolateDiffraction
% INTERPOLATEDIFFRACTION Performs diffraction tomography via interpolation.
%
% This function is called by BACK.
%
% Bradley Ferguson
% The University of Adelaide
% March 2001
%

% read data from the file.
getDPhi;

scale = s*s;

% divide the IFFT by the sampling interval (s*s) to
% properly scale the integral

% the object stores the reconstructed data
Object = zeros(N,N);

% perform the interpolation...
%
for (x = 0:N-1)
    for (y = 0:N-1)
        du = (x-N2)/N/s;
        dv = (y-N2)/N/s;
        [k,l,alpha,beta,rotation] = findray(du,dv,0,M,K,T);

        if (alpha<0)|(alpha>=K+1)|(beta<0)|(beta>M-1)
            Object(x+1,y+1) = 0;
        else
            if (BILINEAR)
                yi1 = alpha - floor(alpha); yi = 1-yi1;
                xi1 = beta - floor(beta); xi = 1-xi1;

                ialpha = floor(alpha) + 1; ibeta = floor(beta)+1;

                if (alpha < K-1)
                    ialpha1 = ialpha+1;
                else
                    ialpha1 = ialpha;
                end

                Object(x+1,y+1) = (Field(ibeta,ialpha)*xi*yi + ...
                    Field(ibeta+1,ialpha)*xi1*yi + Field(ibeta,ialpha1)*xi*yi1 + ...
                    Field(ibeta+1,ialpha1)*xi1*yi1)/scale;
            else
                Object(x+1,y+1)=Field(l,k)/scale;
            end
        end
    end
end

```

B.4 Matlab Code

```
        end
    end
end
end

    if (DEBUG)
        figure(gcf+1);clf;
        imagesc(abs(Object));
        title('Interpolated FFT of Object');
    end

if (lowPass)
    Object = hammingImage(Object,N,1);

    if (DEBUG)
        figure(gcf+1);clf;
        imagesc(abs(Object));
        title('Low pass filtered FFT of Object');
    end
end

% perform the inverse Fourier transform...
Object = modulateImage(Object);
Object = ifft2(Object);
Object = modulateImage(Object);

    if (DEBUG)
        figure(gcf+1);clf;
        imagesc(abs(Object));
        title('Object');
    end



---



function [modulatedImage] = modulateImage(pic)
%     MODULATE
%
%     Modulate a square array of numbers. This is done before
%     taking the FFT of an array to shift the zero frequency to
%     the center of the result array. It is accomplished by
%     multiplying each term of the matrix by  $-1^{(i+j)}$  where
%     i and j are the coordinates of the element.
%
%     Input
%     The address of a square array and its size.
%
%
%     Bradley Ferguson
%     The University of Adelaide
%     March 2002.
%

modulatedImage = pic;
```

```
modulatedImage(1:2:end,2:2:end) = -1*modulatedImage(1:2:end,2:2:end);
modulatedImage(2:2:end,1:2:end) = -1*modulatedImage(2:2:end,1:2:end);
```

```
%      Rytov – Estimate the Complex Phase of a scattered field.
%
%      The estimate of Ub(r) is given by
%                               Us(r)
%      Ub(r) = U0(r) ln (----- + 1)
%                               U0(r)
%
%      This routine transforms one projection. The projection
%      is stored in order in the array (negative then positive).
%
%      Bradley Ferguson
%      The University of Adelaide
%      March 2001
%

U0l0 = exp(j*K0*l0);

Field = Field / U0l0 + 1;

rytovPhase = unwrap(angle(Field));

Field = (log(abs(Field)) + j*rytovPhase)*U0l0; % see (Devaney, 1981)

if (RYTOV_PHASE_FILES)

    ifp = fopen(strcat(ifn, '.phase'), 'r', 'n');
    if (ifp == -1)
        fprintf('Error opening file in <Rytov>\n');
        return;
    end

    [tempField, count] = fread(ifp, 'float32');
    fclose(ifp);

    Field = (log(tempField(1:2:end)-1)/U0l0 + 1) + j*tempField(2:2:end)*U0l0;

% reshape the field
if (~double)
    Field = reshape(Field, M, K);
else
    Field = reshape(Field, M2, K);

% we need to pad the data with zeros...
dField = zeros(M, K);
dField(M4+1:M2+M4, :) = Field;
Field = dField; clear dField;
```

B.4 Matlab Code

```
end

end

if (DEBUG)
    figure(gcf+1); clf;
    subplot(2,1,1);
    imagesc(imag(Field));
    title('Rytov Phase');
    subplot(2,1,2);
    plot(mean(imag(Field),2));
end
```

Classification Functions

```
function [result,featureData] = classificationTesting(theData,nTrain,nTest,...
    feature,classifier,in,order)
% CLASSIFICATIONTESTING This function tests classification
%
% [result] = classificationTesting(theData,nTrain,nTest,feature,classifier,...
%     [in],[order])
%
% This function assumes data of the form:
%     theData = [2*nTrain+2*nTest, L] contains training and testing
%               data for the two classes
%     feature — indicates which feature extraction method to test
%               1. LPC
%               2. FIR poles
%               3. peak amplitude and delay of peak.
%               4. Energy and sum of amplitudes for pulse.
%               5. Use the full signals
%               6. An arbitrary ARX model (orders given by order)
%
%     classifier — the type of classifier to use (if 0 then linear
%                  discriminat analysis is used else type 'help neuralNetwork'
%     in          — is a spare parameter used for feature extraction if
%                  required (eg for LPC, FIR it is the free vector)
%
% Bradley Ferguson
% The University of Adelaide
% August 2002

train1Start = 1;
train1End   = nTrain;
test1Start  = train1End + 1;
test1End    = train1End + nTest;

train2Start = test1End + 1;
train2End   = test1End + nTrain;
test2Start  = train2End + 1;
test2End    = train2End + nTest;
```



```

% generate a set of features based on the data.
if (feature <= 2)

    poleData = zeros(2,size(theData,2));
    zeroData = poleData;
    free = in;

    for vector = 1:size(theData,2)
        % for comparison compile results for 2 pole and 2 zero models.
        Z = iddata(theData(:,vector),free); % the output,input matrix

        if (feature == 1)
            NN = [2 1 0]; % the numbers of poles,~zeros and delays
            th = arx(Z,NN);

            [a,b,c,d,f] = polydata(th);

            % the features are stored in th in the 3rd row.
            poleData(:,vector) = [a(2:3)]';
        else
            NN = [0 2 0]; % the numbers of poles, zeros and delays
            th = arx(Z,NN);

            [a,b,c,d,f] = polydata(th);

            % the features are stored in th in the 3rd row.
            zeroData(:,vector) = b(1:2)';
            featureData = zeroData;
        end
    end

    if (feature == 1)
        featureData = poleData;
        wrong = performClassification(featureData(:,train1Start:train1End), ...
            featureData(:,train2Start:train2End),...
            featureData(:,test1Start:test1End),...
            featureData(:,test2Start:test2End),classifier);

        xlabel('Linear predictor coefficient (a1)');
        ylabel('Linear predictor coefficient (a2)');
        title('Classification training vectors');

        fprintf('Using LPC Coefficients , Classified %i/%i correctly\n',...
            2*nTest-wrong,2*nTest)
    elseif (feature == 2)
        wrong = performClassification(zeroData(:,train1Start:train1End), ...
            zeroData(:,train2Start:train2End),...
            zeroData(:,test1Start:test1End),...
            zeroData(:,test2Start:test2End), classifier);

        xlabel('FIR filter coefficient (b1)');
        ylabel('FIR filter coefficient (b2)');
    end
end

```

B.4 Matlab Code

```
% title('Classification training vectors');

fprintf('Using FIR Coefficients , Classified %i/%i correctly\n',...
        2*nTest-wrong,2*nTest)
end
end

if (feature == 3)

    maxRegions = max(theData);
    [a,delayRegions] = max(theData);
    delayRegions = delayRegions * 4e-14 * 1e12;
    featureData = [maxRegions;delayRegions];

    wrong = performClassification(featureData(:,train1Start:train1End), ...
        featureData(:,train2Start:train2End),...
        featureData(:,test1Start:test1End),...
        featureData(:,test2Start:test2End),classifier);

    xlabel('Maximum amplitude of THz response (a.u.)');
    ylabel('Delay of maximum peak in THz response (ps)');
    title('Classification training vectors');

    fprintf('Using Max amplitude , Classified %i/%i correctly\n',2*nTest-wrong,2*nTest)
end

if (feature == 4)

    energyRegions = sum(abs(theData).^2,1);
    sumRegions = sum(abs(theData),1);
    featureData = [energyRegions;sumRegions];

    wrong = performClassification(featureData(:,train1Start:train1End), ...
        featureData(:,train2Start:train2End),...
        featureData(:,test1Start:test1End),...
        featureData(:,test2Start:test2End),classifier);

    xlabel('Energy in THz response (a.u.)');
    ylabel('Sum of amplitude of THz response (ps)');
    title('Classification training vectors');

    fprintf('Using Energy , Classified %i/%i correctly\n',2*nTest-wrong,2*nTest)

end

if (feature == 5)
    featureData = theData;

    wrong = performClassification(featureData(:,train1Start:train1End), ...
        featureData(:,train2Start:train2End),...
        featureData(:,test1Start:test1End),...
        featureData(:,test2Start:test2End),classifier);
```

```

    fprintf('Using Full Signals , Classified %i/%i correctly\n',2*nTest-wrong,2*nTest)

end

if (feature == 6)
    free = in;

    featureData = zeros((order(1)+order(2)+order(3)),size(theData,2));
    size(featureData);

    for vector = 1:size(theData,2)

        Z = iddata(theData(:,vector),free); % the output,input matrix

        NN = order;
        th = arx(Z,NN);

        [a,b,c,d,f] = polydata(th);
        size([a(2:end),b,c(2:end)]');
        [a(2:end),b,c(2:end)]';
        featureData(:,vector) = [a(2:end),b,c(2:end)]';
    end

    wrong = performClassification(featureData(:,train1Start:train1End), ...
        featureData(:,train2Start:train2End),...
        featureData(:,test1Start:test1End),...
        featureData(:,test2Start:test2End),classifier);

    fprintf('Using ARX Model Coefficients , Classified %i/%i correctly\n',...
        2*nTest-wrong,2*nTest)

end

result = wrong;

```

```

function [misclassified] = performClassification(class1Train,class2Train,...
    class1,class2,classificationType)
% PERFORMCLASSIFICATION Classifies the inputs using the training vectors.
%
% [misclassified] = performClassification(class1Train,class2Train, ...
%     class1, class2, classificationType)
%
% A classifier is trained on class1Train and class2Train
% and then tested on class1 and class2 (the data for each sample
% must be in the rows of these matrices.. classificationType determines
% the type of network.
% 0 = Mahanolobis distance)
% 1 = perceptron
% 2 = linear neuron
% 3 = 2 layer probalistic neural network.
%

```

B.4 Matlab Code

```
% Bradley Ferguson
% The University of Adelaide
% May 2001
%

if (classificationType > 0)
    neuralNetwork(class1Train , class2Train , class1 , class2 , classificationType);
else
    % use the matlab function 'classify'.

    % the training data
    P = [ class1Train , class2Train ];

    % the classifications for the training data
    C = [ ones(1 , size(class1Train , 2)) , 2*ones(1 , size(class2Train , 2)) ];

    % display this data
    % plotpv(P,C);

    % the test data
    T = [ class1 , class2 ];

    [A] = classify(T' , P' , C' , 'mahalanobis');

    misclas1 = find(A(1:length(class1))~=1);
    misclas2 = find(A(length(class1)+1:end)~=2);
    clas1 = find(A(1:length(class1))==1);
    clas2 = find(A(length(class1)+1:end)==2);

    if (size(class1Train , 1) <= 3)
        clf
        hold on

        useColor = 1;
        justPrintTraining = 1;
        if (useColor == 1)
            if (justPrintTraining == 1)
                plot(class1Train(1,:) , class1Train(2,:) , 'bx');
                plot(class2Train(1,:) , class2Train(2,:) , 'ro');
            else
                plot(class1Train(1,:) , class1Train(2,:) , 'bx');
                plot(class2Train(1,:) , class2Train(2,:) , 'bo');
                plot(class1(1,clas1) , class1(2,clas1) , 'gx');
                plot(class1(1,misclas1) , class1(2,misclas1) , 'rx');
                plot(class2(1,clas2) , class2(2,clas2) , 'go');
                plot(class2(1,misclas2) , class2(2,misclas2) , 'ro');
            end
        else
            plot(class1Train(1,:) , class1Train(2,:) , 'o');
            plot(class2Train(1,:) , class2Train(2,:) , 'x');
            plot(class1(1,clas1) , class1(2,clas1) , 'o');
            plot(class1(1,misclas1) , class1(2,misclas1) , 'o');
            plot(class2(1,clas2) , class2(2,clas2) , 'x');
```

```

        x = plot(class2(1,misclas2),class2(2,misclas2),'x');
        set(x)
    end

    end

end

misclassified = length(misclas1)+length(misclas2);

% confusion matrix:
confusionM = [length(clas1),length(misclas1);length(misclas2),length(clas2)]



---



function [confusionMatrix,accuracy] = pcaClassification(numTrain,numTest,C1,C2,C3)
% PCACLASSIFICATION Uses PCA to classify the input data classes
%
% [confusionMatrix,accuracy] = pcaClassification(numTrain,numTest,C1,C2,C3)
%
% Principal Component Analysis is used to classify the three input
% classes defined in C1, C2 and C3.
% Half the data is used to train a classifier, the other half is used
% to test the resultant classifier. The resultant confusionMatrix and
% classifier accuracy are returned.
%
% Bradley Ferguson
% The University of Adelaide
% March 2003
%

% try to classify the 3 classes using a KL (PCA) based technique
% for feature extraction.
%

theDataTrain = [C1(:,1:2:end),C2(:,1:2:end),C3(:,1:2:end)];
theDataTest = [C1(:,2:2:end),C2(:,2:2:end),C3(:,2:2:end)];

[eigenVecs,zScores,pcaVals,tsquare] = princomp(theDataTrain');
meanDataTrain = mean(theDataTrain,2);

figure(gcf+1);clf;
subplot(3,1,1);
plot(time,eigenVecs(:,1));
formatImage(1);
title('(a)');
subplot(3,1,2);
plot(time,eigenVecs(:,2));
formatImage(1);
title('(b)');
ylabel('Normalised amplitude (a.u.)');
subplot(3,1,3);

```

B.4 Matlab Code

```
plot(time,eigenVecs(:,3));
formatImage(1);
title('(c)');
xlabel('time (ps)');

if (printPlots == 1)
    print(printOpts, strcat(savePath, 'pcaVecs'));
end

figure(gcf+1);clf;subplot(2,1,1);
plot(10*log10(pcaVals(1:10)/pcaVals(1)));
formatImage(1);
xlabel('Eigenvalue');
ylabel('Amplitude (dB)');

if (printPlots == 1)
    print(printOpts, strcat(savePath, 'pcaVals'));
end

% now project the data onto the first N eigenvectors and use the
% eigen values as features for classification
%

meanDataTrain = repmat(meanDataTrain,1,size(theDataTest,2));

testCoeffs = (theDataTest-meanDataTrain)' * eigenVecs(:,1:50);
trainCoeffs = (theDataTrain-meanDataTrain)' * eigenVecs(:,1:50);
size(testCoeffs);

figure(gcf+1);clf;

plot(testCoeffs(1:numTest,1)/max(max(testCoeffs)),...
      testCoeffs(1:numTest,2)/max(max(testCoeffs)), 'bo');
hold on;
plot(testCoeffs(numTest+1:2*numTest,1)/max(max(testCoeffs)),...
      testCoeffs(numTest+1:2*numTest,2)/max(max(testCoeffs)), 'rs');
plot(testCoeffs(2*numTest+1:end,1)/max(max(testCoeffs)),...
      testCoeffs(2*numTest+1:end,2)/max(max(testCoeffs)), 'g>');

formatImage(1);
xlabel('Projection onto eigenvector 1');
ylabel('Projection onto eigenvector 2');
legend('C1','C2','C3');

if (printPlots == 1)
    print(printOpts, strcat(savePath, 'scatterPCA1and2'));
end

figure(gcf+1);clf;

plot(testCoeffs(1:numTest,3)/max(max(testCoeffs)),...
      testCoeffs(1:numTest,4)/max(max(testCoeffs)), 'bo');
```

```

hold on;
plot(testCoeffs(numTest+1:2*numTest,3)/max(max(testCoeffs)),...
      testCoeffs(numTest+1:2*numTest,4)/max(max(testCoeffs)), 'rs');
plot(testCoeffs(2*numTest+1:end,3)/max(max(testCoeffs)),...
      testCoeffs(2*numTest+1:end,4)/max(max(testCoeffs)), 'g>');

formatImage(1);
xlabel('Projection onto eigenvector 3');
ylabel('Projection onto eigenvector 4');
legend('C1','C2','C3');

if (printPlots == 1)
    print(printOpts, strcat(savePath, 'scatterPCA3and4'));
end

numVecs = 12; % the number of eigenvectors to use for feature extraction

T = [testCoeffs(:,1:numVecs)];
S = [trainCoeffs(:,1:numVecs)];
G = [ones(1,numTrain),2*ones(1,numTrain),3*ones(1,numTrain)]';

classX = classify(S,T,G, 'mahalanobis');
[confusionMatrix,accuracy] = calcConfusionMatrix(classX,numTest)



---


function [confusionMatrix,accuracy] = calcConfusionMatrix(classX,numTest)
% CALCONFUSIONMATRIX Calculates the confusion matrix given classification
%           results
%
% function confusionMatrix = calcConfusionMatrix(classX,numTest)
%
% Bradley Ferguson
% The University of Adelaide
% March 2003

numClasses = length(classX)/numTest;
confusionMatrix = zeros(numClasses);

for i = 1:numClasses
    for j = 1:numClasses
        confusionMatrix(j,i) = length(find(classX((i-1)*numTest+1:i*numTest) == j));
    end
end

accuracy = trace(confusionMatrix) / length(classX);

confusionMatrix = confusionMatrix / numTest;

```

B.4 Matlab Code

THz Pre-processing Functions

```
function unwrappedMatrix = myUnwrap(inputMatrix , deltaF , lowerExtBound , upperExtBound)
% MYUNWRAP Unwraps the frequency data by extrapolating to low frequency.
%
%     unwrappedMatrix = myUnwrap(inputMatrix , deltaF , lowerExtBound , upperExtBound)
%
%     This function prevents phase unwrapping problems by using the
%     a dispersionless approximation to unwrap the phase of the complex
%     array 'inputMatrix' for low frequencies below 'lowerExtBound'.
%     The phase between 'upperExtBound' and 'lowerExtBound' is used to
%     estimate the linear phase to be extrapolated.
%     'deltaF' provides the frequency resolution of the input array.
%
%     Bradley Ferguson
%     The University of Adelaide
%     February 2003

% first unwrap normally.
x = unwrap(angle(inputMatrix));

% now extrapolate the low frequency data.
lowerExtBoundIndex = ceil(lowerExtBound / deltaF); % 0.4 THz
upperExtBoundIndex = floor(upperExtBound / deltaF); % 0.8 THz

averageSlope = mean(diff(x(lowerExtBoundIndex:upperExtBoundIndex ,: ,: ,:)));

x(1:lowerExtBoundIndex - 1 ,: ,: ,:) = repmat([0:(lowerExtBoundIndex - 2)]' , ...
    [1 , size(x,2) , size(x,3) , size(x,4)]) * repmat(averageSlope , ...
    [lowerExtBoundIndex - 1 , 1 , 1 , 1]);
x(lowerExtBoundIndex:end ,: ,: ,:) = x(lowerExtBoundIndex:end ,: ,: ,:) - ...
    repmat(x(lowerExtBoundIndex ,: ,: ,:) , [ size(x,1) - lowerExtBoundIndex + 1 , 1 , 1 , 1]) + ...
    (lowerExtBoundIndex - 1) * repmat(averageSlope , ...
    [ size(x,1) + 1 - lowerExtBoundIndex , 1 , 1 , 1]);

unwrappedMatrix = x;



---


function [deconMag , deconPhase , deconTime , freqStep] = deconvolve(sample , ref , ...
    timeStep , padFactor , overSamplein , removeOffsetin , debugPlot , postProcessPhaseIn)
% DECONVOLVE deconvolves a signal using a reference signal.
%     [deconMag , deconPhase , deconTime , freqStep] = deconvolve(sample , ref , timeStep , ...
%         padFactor , overSample , removeOffset , debugPlot , postProcessPhase)
%
%     This function deconvolves the signal by dividing the Fourier
%     transforms of the two signals. The padfactor allows the FFTs
%     to be zero padded to interpolate (and improve the phase unwrapping)
%     The magnitude and phase of the deconvolved signal in the Fourier
%     domain are returned along with the complex time domain signal.
%
%     debugPlots allows plots to be generated.
%
%     Bradley Ferguson
```



```

% The University of Adelaide
% July 2001
%

if (nargin >= 5)
    overSample = overSamplein;
else
    overSample = 0;
end;

if (nargin >= 6)
    removeOffset = removeOffsetin;
else
    removeOffset = 0;
end;

if (nargin >= 7)
    printPlots = debugPlot;
else
    printPlots = 0;
end;

if (nargin >= 8)
    postProcessPhase = postProcessPhaseIn;
else
    postProcessPhase = 1;
end;

% first remove the dc offset on the signals.
if (removeOffset == 1)
    ref = ref - mean(ref);
    sample = sample - mean(sample);
end

% the length 'l' of the deconvolved signal is the
% minimum length of the input vectors.
refL = length(ref);
sampL = length(sample);
l = min(refL,sampL);
time = [1:l]*timeStep;

pfreqL = l*padFactor;
prefFFT = fft(ref,pfreqL);
psampFFT = fft(sample,pfreqL);

freq = [0:pfreqL]'/pfreqL/timeStep;
freqStep = 1/pfreqL/timeStep;

pdeconFFT = psampFFT ./ prefFFT;

% set the first value of the deconvolved signal to 0
% pdeconFFT(1)

```

B.4 Matlab Code

```
pdeconFFT(1) = 0;

deconTime = ifft(pdeconFFT);

if 1 == 1
    psampPhase = myUnwrap(psampFFT, freqStep/1e12, .2, .5);
    prefPhase = myUnwrap(prefFFT, freqStep/1e12, .2, .5);
else
    psampPhase = unwrap(angle(psampFFT));
    prefPhase = unwrap(angle(prefFFT));

    % if post process phase
    if (postProcessPhase == 1)
        % calculate the sample range corresponding to 0.2–0.4 THz.
        linearLowerFreq = 0.1e12;
        linearUpperFreq = 0.2e12;
        sampleRange = [ceil(linearLowerFreq / freqStep) : ...
            ceil(linearUpperFreq / freqStep)];
        phaseSlopeSamp = mean(diff(psampPhase(sampleRange)));
        phaseSlopeRef = mean(diff(prefPhase(sampleRange)));

        % now assume the phase is linear below the lower limit
        psampPhase(1:sampleRange(1)-1) = phaseSlopeSamp * [0:sampleRange(1)-2];
        psampPhase(sampleRange(1):end) = psampPhase(sampleRange(1):end) - ..
            psampPhase(sampleRange(1)) + ...
                phaseSlopeSamp * (sampleRange(1)-1);

        prefPhase(1:sampleRange(1)-1) = phaseSlopeRef * [0:sampleRange(1)-2];
        prefPhase(sampleRange(1):end) = prefPhase(sampleRange(1):end) - ...
            prefPhase(sampleRange(1)) + ...
                phaseSlopeRef * (sampleRange(1)-1);
    end
end

deconPhase = psampPhase - prefPhase;
pdeconMag = abs(pdeconFFT);

if (overSample == 1)
    deconMag = pdeconMag;
else
    % subsample the phase to get back to the normal number of samples
    deconMagPad = pdeconMag;
    deconMag = pdeconMag(1:padFactor:end);
    deconPhasePad = deconPhase;
    deconPhase = deconPhase(1:padFactor:end);
    freqStepPad = freqStep;
    freqStep = freqStep*padFactor;
end

if (printPlots==1)

    freqCutoff = min(ceil(4e12/freqStepPad), ceil(padFactor*1/2));
```

```

figure(gcf+1); clf;
plot(time,ref)
hold on
plot(time,sample,'r');
formatImage(2)
title('THz signals');
xlabel('time (ps)');
legend('Reference','Sample');

figure(gcf+1); clf;
plot(freq(1:freqCutoff),log10(abs(prefFFT(1:freqCutoff))));
hold on
plot(freq(1:freqCutoff),log10(abs(psampFFT(1:freqCutoff))),'r');
plot(freq(1:freqCutoff),log10(abs(pdeconFFT(1:freqCutoff))),'g');
formatImage(2)
title('THz spectrums');
xlabel('freq (THz)');
legend('Reference','Sample','Deconvolved');

figure(gcf+1); clf;
plot(time,abs(deconTime(1:length(time))));
formatImage(2)
xlabel('time (ps)');
title('deconvolved signal');

figure(gcf+1); clf;
subplot(2,1,1);
plot(freq(1:freqCutoff),deconPhasePad(1:freqCutoff));
subplot(2,1,2);
plot(freq(1:freqCutoff),deconMagPad(1:freqCutoff));
formatImage(2)
title('magnitude and phase of deconvolved signal');

figure(gcf+1); clf;
plot(freq(1:freqCutoff),psampPhase(1:freqCutoff));
hold on; plot(freq(1:freqCutoff),prefPhase(1:freqCutoff),'r');
plot(freq(1:freqCutoff),deconPhasePad(1:freqCutoff),'g');
formatImage(2)
title('phase of ffts');
xlabel('frequency(Hz)');
end

```

Refractive Index Estimation

```

function [nVector,freqVector,errorVector] = nNelderMead(sample,reference,...
    samplePeriod,FP,thickness,nsubstin,zeroPadin,removeOffsetin,holderin,debugPlots)
% nNelderMead Calculates the complex refractive index
%
% [nVector,freqVector,errorVector] = nNelderMead(sample,reference,samplePeriod,FP,...
%     thickness,[nsubst,zeroPad,removeOffset,holder,debug])

```

B.4 Matlab Code

```
%
% This function uses the Nelder Mead method to iteratively calculate the
% frequency dependent refractive index of a sample given a sample and reference
% THz pulse.
% If FP = 1 the Fabry Perot effect is taken into account.
% zeroPad determines how much the signals are padded before taking the
% Fourier transform. This can improve the accuracy of the
% phase unwrapping but it can also introduce spikes in the
% amplitude plot.
%
%
% Bradley Ferguson
% The University of Adelaide
% July 2001

global f_nsubst f_omega f_L f_clight f_FP f_magMeas f_phaseMeas f_freq ...
       f_freqIndex f_phaseHolder f_magHolder

if (nargin >= 5)
    L = thickness;
else
    L = 508e-6; % the length of the sample
end

if (nargin >= 6)
    nsubst = nsubstin;
else
    nsubst = 1.00027;
end

% zeroPad determines how much the signals are padded before taking the
% Fourier transform. This can improve the accuracy of the
% phase unwrapping but it can also introduce spikes in the
% amplitude plot.
%
if (nargin >= 7)
    zeroPad = zeroPadin;
else
    zeroPad = 1;
end

if (nargin >= 8)
    removeOffset = removeOffsetin;
else
    removeOffset = 1;
end

if (nargin >= 9)
    holder = holderin;
else
    holder = 0;
end
```

```

if ( nargin >= 10)
    debugPlot = debugPlots;
else
    debugPlot = 0;
end

f_clight = 3e8;
f_L = L;
f_FP = FP;
f_nsubst = nsubst;

minFreq = .3e12;
maxFreq = 2.1e12;
numFreqSteps = 400;

expectedN = 3.2;
expectedK = 0.00;

freqCounter = 0;

% perform simulation using estimate results.
if 1==0
    simComp(sample,reference,samplePeriod,L,expectedN,expectedK,nsubst,FP,1);
end %1==0

% the measured T is determined by simple deconvolution.
[deconMag,deconPhase,deconTime,freqStep] = deconvolve(sample,reference,...
    samplePeriod,zeroPad,0,removeOffset,0);

f_freq = [1:length(deconMag)]*freqStep; % the frequency vector
minFreqIndex = floor(minFreq/freqStep)+1;
maxFreqIndex = floor(maxFreq/freqStep)+1;
freqIndexStep = floor((maxFreqIndex-minFreqIndex)/numFreqSteps);
if freqIndexStep == 0
    freqIndexStep = 1;
end

numFreqSteps = ceil((maxFreqIndex-minFreqIndex)/freqIndexStep);
maxFreqIndex = minFreqIndex + numFreqSteps*freqIndexStep;

nVector = zeros((maxFreqIndex-minFreqIndex)/freqIndexStep,1);
freqVector = nVector;
errorVector = nVector;

currentPoint = [expectedN,expectedK];

% If a holder is used for the sample then Fabry Perot corrections must be
% applied to the reference response as well. Calculate this correction
f_magHolder = ones(size(f_freq));

```

B.4 Matlab Code

```
f_phaseHolder = zeros(size(f_freq));

if (FP==1)
    if (holder == 1)
        fprintf('Calculating Holder correction\n');
        n_holder = 1;
        [f_magHolder,f_phaseHolder] = calcHolderCorrection(n_holder,f_freq,f_L,...
            f_clight,f_nsubst,1);
    end
end

nmOptions = optimset('display','off'); %,'MaxIter','1000*numberOfVariables',...
%      'MaxFunEvals','1000*numberOfVariables','TolFun',1e-8,'TolX',1e-6);

% for each frequency iteratively solve for n_complex
for freqIndex = minFreqIndex:freqIndexStep:maxFreqIndex
    freqCounter = freqCounter + 1;
    f_omega = f_freq(freqIndex) * 2 * pi;
    f_magMeas = deconMag(freqIndex);
    f_phaseMeas = abs(deconPhase(freqIndex));
    f_freqIndex = freqIndex;

    % currentPoint = [expectedN,expectedK];

    % calculate the point using fminsearch
    [nextPoint,f_error,exitFlag] = fminsearch('duvill96Error',currentPoint,nmOptions);

    if (exitFlag ==1)
        currentPoint = nextPoint;
    else
        % if the fminsearch was unable to converge simply use the previous value
    end

    nVector(freqCounter) = currentPoint(1)+j*currentPoint(2);
    freqVector(freqCounter) = f_freq(freqIndex);
    errorVector(freqCounter) = f_error;

    if (1==0) % optional code used during testing.
        absT = calcAbsT(expectedN,expectedK,nsubst,f_omega,L,f_clight,FP);
        argT = calcArgT(expectedN,expectedK,nsubst,f_omega,L,f_clight,FP);
        modAbsT = calcAbsT(currentPoint(1),currentPoint(2),...
            nsubst,f_omega,L,f_clight,FP);
        modArgT = calcArgT(currentPoint(1),currentPoint(2),...
            nsubst,f_omega,L,f_clight,FP);

        fprintf('magnitude: measured: %f should be: %f modelled: %f\n',...
            f_magMeas,absT,modAbsT);
        fprintf('phase: measured: %f should be: %f modelled: %f\n',...
            f_phaseMeas,argT,modArgT);
    end % 1==1
```

```

end % for loop

if debugPlot==1
    figure(gcf+1);
    clf;
    subplot(2,1,1);
    plot(freqVector/1e12,real(nVector));
    f = findobj(gcf,'LineWidth',0.5);
    set(f,'LineWidth',2);
    g = findobj(gcf,'fontsize',10);
    set(g,'fontsize',16);
    set(gca,'fontsize',16);

    ylabel('n');
    hold on
    grid on;

    % plot(freqVector/1e12,ones(size(freqVector))*expectedN,'r');
    subplot(2,1,2);
    plot(freqVector/1e12,imag(nVector));
    f = findobj(gcf,'LineWidth',0.5);
    set(f,'LineWidth',2);
    g = findobj(gcf,'fontsize',10);
    set(g,'fontsize',16);
    set(gca,'fontsize',16);

    ylabel('k');
    xlabel('frequency (THz)');
    grid on;

end

```

```

function [deconAbs,deconPhase,simAbs,simPhase] = simComp(sample,reference,...
    samplePeriod,L,n,k,nsubst,FP,debugPlot)
% SIMCOMP compares simulated results with deconvolved responses.
% [deconAbs,deconPhase,simAbs,simPhase] = simComp(sample,reference,samplePeriod,...
%     L,n,k,nsubst,FP,debugPlot)
%
% This function simulates the response assuming 0 dispersion.
%
% Bradley Ferguson
% The University of Adelaide
% July 2001
%

if (nargin >=9)
    genPlots = debugPlot;
else
    genPlots = 0;
end
clight = 3e8;

```

B.4 Matlab Code

```
[deconMag,deconPhase,deconTime,freqStep] = deconvolve(sample,reference,...
    samplePeriod,1,1);

deconPhase = abs(deconPhase);

freq = [1:length(deconMag)]*freqStep; % the frequency vector

% now calculate the simulated mag and phase

simMag = calcAbsT(n,k,nsubst,2*pi*freq,L,clight,FP);
simPhase = calcArgT(n,k,nsubst,2*pi*freq,L,clight,FP);

if (genPlots == 1)
    freqCutoff = ceil(2e12/freqStep);
    figure(gcf+1)
    clf;
    plot(freq(1:freqCutoff)/1e12,deconMag(1:freqCutoff));
    hold on;
    plot(freq(1:freqCutoff)/1e12,simMag(1:freqCutoff),'r');
    formatImage(2);
    legend('measured','simulated');
    title('Simulated and Measured Amplitude');

    figure(gcf+1)
    clf;
    plot(freq(1:freqCutoff)/1e12,deconPhase(1:freqCutoff));
    hold on;
    plot(freq(1:freqCutoff)/1e12,simPhase(1:freqCutoff),'r');
    formatImage(2);
    legend('measured','simulated');
    title('Simulated and Measured Phase');

end

function [magMeasFP,phaseMeasFP] = fp_T_meas(magMeas,phaseMeas,n_FP,freq,L,...
    clight,freqIndex,nsubst,fastModein)
% FP_T_MEAS modifies the measured T based on the FP effect
% [magMeas,phaseMeas] = fp_T_meas(magMeas,phaseMeas,n_fp,freq,L,clight,...
%     freqIndex,nsubst,fastModein)
%
% This function divides the measured T by the T calculated for the
% Fabry Perot effect.
%
% Bradley Ferguson
% The University of Adelaide
% July 2001
%
```

```

if (nargin >= 9)
    fastMode = fastModein;
else
    fastMode = 0;
end

if (fastMode == 1)
    freq = freq(freqIndex);
    freqIndex = 1;
end

% note: special test mode assumes there is only 1 reflection
if (FP == 2)

    fpCoeff = ones(size(freq)) / (((n_FP - nsubst)/(n_FP + nsubst))^2 * ...
        exp(-2*j*n_FP*2*pi*freq*L/clight) + 1);
    f_magFP = (abs(fpCoeff));
    f_phaseFP = unwrap(angle(fpCoeff));

elseif (FP == 1)
    fpCoeff = ones(size(freq)) - ((n_FP - nsubst)/(n_FP + nsubst))^2 * ...
        exp(-2*j*n_FP*2*pi*freq*L/clight);

    f_magFP = (abs(fpCoeff));
    f_phaseFP = unwrap(angle(fpCoeff));
end

magMeasFP = magMeas / f_magFP(freqIndex);
phaseMeasFP = abs(phaseMeas) - f_phaseFP(freqIndex);

```

```

function [magMeasFP, phaseMeasFP] = calcHolderCorrection(n_FP, freq, L, ...
    clight, nsubst, plotDebug)
% CALCHOLDERCORRECTION calculates correction factors for a sample holder
% [magMeas, phaseMeas] = calcHolderCorrection(n_FP, freq, L, clight, nsubst)
%
% This function calculates correction factors for the magnitude and
% phase, when multiple reflections arise from the sample holder.
%
% Bradley Ferguson
% The University of Adelaide
% July 2001
%

if (nargin >= 6)
    printPlot = plotDebug;
else
    printPlot = 0;
end

f_magFP = (abs(ones(size(freq)) - ((n_FP - nsubst)/(n_FP + nsubst))^2 * ...

```

B.4 Matlab Code

```
exp(-2*j*n_FP*2*pi*freq*L/clight));
f_phaseFP = unwrap(angle(ones(size(freq))-((n_FP - nsubst)/(n_FP + nsubst))^2*...
exp(-2*j*n_FP*2*pi*freq*L/clight)));

magMeasFP = f_magFP;
phaseMeasFP = f_phaseFP;

if (printPlot==1)
    figure(11); clf;
    subplot(2,1,1)
    plot(magMeasFP);

    subplot(2,1,2);
    plot(phaseMeasFP);

end

function theError = duvill96Error(currentPoint)
% DUVILL96ERROR calculates the error in the (Duvillaret 1996) model
% theError = duvill96Error(currentPoint)
%
% This function calculates arg(T) based on the formula in duvill99
%
% Bradley Ferguson
% The University of Adelaide
% July 2001
%

global f_nsubst f_omega f_L f_clight f_FP f_magMeas f_phaseMeas f_freq ...
f_freqIndex f_phaseHolder f_magHolder

n = currentPoint(1);
k = currentPoint(2);

argT = ((n-1)*f_omega*f_L/f_clight + atan(k/(n*(n+f_nsubst)+k^2)));

absT = 2*2*f_nsubst*sqrt(n^2+k^2)*exp(-1*k*f_omega*f_L/f_clight)/((n+f_nsubst)^2+k^2);

if (f_FP == 1)
    n_FP = currentPoint(1) - j*currentPoint(2);

    [fp_magMeas,fp_phaseMeas] = fp_T_meas(f_magMeas,f_phaseMeas,n_FP,...
f_freq,f_L,f_clight,f_freqIndex,f_nsubst,1);

    theError = (absT*f_magHolder(f_freqIndex) - fp_magMeas)^2 + ...
    (argT+f_phaseHolder(f_freqIndex) - fp_phaseMeas)^2;
```

```
else
```

```
    theError = (absT - f_magMeas)^2 + (argT - f_phaseMeas)^2;
```

```
end
```

Appendix C

Refractive Index Extraction

The early motivation for THz-TDS was for semiconductor characterisation (van Exter and Grischkowsky 1990c, van Exter and Grischkowsky 1990a). These systems remain most useful for the study of thin planar materials including semiconductors, thin films (Li et al. 1999a, Jiang et al. 2000a), and superconductors (Shikii et al. 1999, Tonouchi et al. 2000). The broadband coherent nature of THz-TDS measurements allow the complex refractive index of the sample to be extracted over the spectral range from 100 GHz up to 5 THz. However, the extraction of the material properties from the THz pulse measurements is not always straightforward. The complication arises from reflections of the THz pulse at the material boundaries. This can lead to multiple reflections in the measured response.

If the material is thick enough to allow these reflections to be isolated, and two samples of the material with differing thickness are available, then the material parameters can be easily extracted through a Fourier domain ratio. In a more general case, advanced algorithms are required. This Appendix presents the general procedure for material parameter extraction as adopted in this Thesis. It follows the work of Duvillaret et al. (1996).

C.1 Problem Geometry

Figure C.1 defines the geometry for a standard THz-TDS experiment. First the THz response of the system is measured without the sample, E_r . The sample consists of a planar slab of material with thickness l , with parallel plane surfaces perpendicular to the THz beam path. The sample is assumed to be magnetically isotropic and there are no surface charges. If the material is birefringent the polarisation of the THz beam is assumed to be parallel to the optical axis of the material. The material is characterised by the frequency dependent, complex refractive index $\tilde{n}(\omega)$. The measured THz signal

C.1 Problem Geometry

after transmission through the sample is given by the sum of the transmitted radiation and an infinite sum of Fabry-Perot reflections.

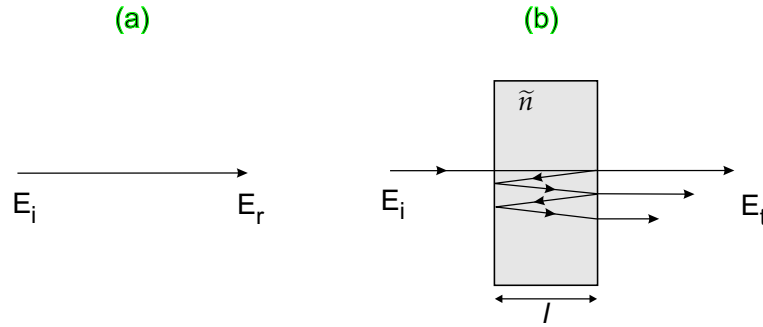


Figure C.1. Sample geometry for a typical THz-TDS experiment. (a) The incident THz beam, E_i is measured without the sample in place. This is referred to as the reference or ‘free air’ response and is denoted E_r . (b) A planar slab of the target material with thickness l is placed in the THz beam path, perpendicular to the beam propagation direction. The measured signal consists of the transmitted portion of the incident beam and reflections arising from multiple transversals of the sample. The measured signal is denoted E_t . After (Duvillaret et al. 1996).

The refractive index of air is assumed to be $1 + i0$. In the frequency, ω , domain the sample response $E_t(\omega)$ is given by

$$E_t(\omega) = \frac{4\tilde{n}}{(\tilde{n} + 1)^2} \exp \left[-i \frac{\tilde{n}\omega l}{c} \right] \cdot \sum_{k=0}^{\infty} \left\{ \frac{\tilde{n} - 1}{\tilde{n} + 1} \cdot \exp \left[-i \frac{\tilde{n}\omega l}{c} \right] \right\}^{2k} \cdot E_i(\omega), \quad (\text{C.1})$$

where $E_i(\omega)$ is the incident THz field, c is the speed of light and $\tilde{n} = n(\omega) + i\kappa(\omega)$ and the frequency dependence has been omitted for notational simplicity. The complex transmission coefficient $T(\omega)$ is calculated by dividing the sample response, $E_t(\omega)$, by the reference response, $E_r(\omega)$, in the frequency domain. The noise robustness of this deconvolution procedure can be improved by the techniques discussed in Ch. 5, but in the simplest case

$$T(\omega) = \frac{E_t(\omega)}{E_r(\omega)} = \frac{4\tilde{n}}{(\tilde{n} + 1)^2} \exp \left[-i \frac{(\tilde{n} - 1)\omega l}{c} \right] \cdot \left\{ \frac{1}{1 - \left(\frac{\tilde{n} - 1}{\tilde{n} + 1} \right)^2 \cdot \exp \left[-2i \frac{\tilde{n}\omega l}{c} \right]} \right\}. \quad (\text{C.2})$$

In the majority of cases the sample is *optically thick*, which implies that the THz pulse echoes caused by multiple reflections are temporally well separated. In this case the

measured THz signal may be windowed to isolate the main pulse and Eq. (C.2) is simplified. The term on the right becomes equal to 1, because all reflection terms are omitted, and

$$T(\omega) = \frac{E_t(\omega)}{E_r(\omega)} = \frac{4\tilde{n}}{(\tilde{n}+1)^2} \exp \left[-i \frac{(\tilde{n}-1)\omega l}{c} \right]. \quad (\text{C.3})$$

Analytic solutions for Eqs. (C.2) and (C.3) do not exist, and these equations are typically solved using numerical techniques. Duvillaret et al. (1996) described an iterative method for solving Eq. (C.3) based on minimising an error function $\epsilon(n, \kappa)$ defined in terms of the log amplitude and argument of $T(\omega)$, where n and κ are the real and imaginary parts of the complex refractive index $\tilde{n}$.

$$\epsilon(n, \kappa) = \delta\rho^2 + \delta\varphi^2, \quad (\text{C.4})$$

where

$$\delta\rho = \ln |T(\omega)| - \ln |T_{\text{meas}}(\omega)|, \quad (\text{C.5})$$

and

$$\delta\varphi = \arg \{T(\omega)\} - \arg \{T_{\text{meas}}(\omega)\}, \quad (\text{C.6})$$

given the measured value of $T(\omega)$ denoted $T_{\text{meas}}(\omega)$ and the calculated value of $T(\omega)$ given the current estimate of $n(\omega)$ and $\kappa(\omega)$. Note that ϵ is a smooth quadratic function in n and κ and its minimum may be found using established numeric techniques such as the Nelder-Mead simplex method (Nelder and Mead 1965). Duvillaret et al. (1996) showed that this method generally converged within 2 and 3 iterations for optically thick samples. For optically thin samples an additional processing stage was proposed by Duvillaret et al. (1996). The term on the right of Eq. (C.2) was denoted $A_{\text{FP}}(\omega)$ such that

$$A_{\text{FP}}(\omega) = \frac{1}{1 - \left(\frac{\tilde{n}-1}{\tilde{n}+1} \right)^2 \cdot \exp \left[-2i \frac{\tilde{n}\omega l}{c} \right]}. \quad (\text{C.7})$$

This term is treated as a perturbation to the basic equation Eq. (C.3). Initial estimates of n and κ are used to estimate the value of $A_{\text{FP}}(\omega)$. This term is multiplied by the measured $T_{\text{meas}}(\omega)$ to reduce the multiple reflections and the same procedure used for optically thick samples is applied to refine the estimate of n and κ . Repeating this procedure was shown to converge on the accurate material parameters in few iterations.

A number of points are worth highlighting.:

1. In the case of optically thin samples Eq. (C.2) is only accurate if *all* multiple reflections are measured. In theory this requires measuring the THz pulse over infinite time. In practice the amplitude of the reflections will quickly drop below the noise floor for most practical samples. In the case where a known, fixed number of reflections are measured Eq. (C.2) may be modified to incorporate the specific number of reflections as shown by (Dorney et al. 2001a).
2. Additionally, using the phase of the transmission function as part of the error function Eq. (C.4) necessitates accurate phase unwrapping. This issue is discussed in detail in Sec. 4.6.5 of Ch. 4.
3. A common variation on the problem described in Fig. C.1 is one where the target material is either a thin film on the surface of a substrate material, or is suspended in a holder of some description (an example is the teflon holder shown in Ch. 5 Fig. 5.30). Duvillaret et al. (1996) derived a general formulation that is very similar to that presented above, and encompasses these cases. The only modifications required are to measure the reference THz pulse through the substrate or holder and to incorporate the refractive index of this material in Eq. (C.2) instead of that of air (1).
4. Finally, this algorithm requires *a priori* knowledge of the material thickness l . More complicated algorithms for independent extraction of both thickness and refractive index have also been proposed (Duvillaret et al. 1999, Dorney et al. 2001a).

Appendix D

Radon's Inversion Formula

A solution for straight line tomographic reconstruction has existed since 1917. Radon (1917) derived an explicit inversion formula for the Radon transform that, in theory, allows an object to be reconstructed from its projections. However, his formula encountered a number of practical difficulties, which prevented it from ever being used experimentally. Fifty years later the filtered backprojection algorithm overcame most of these difficulties and revolutionised the field of medical tomographic imaging. The filtered backprojection algorithm forms the basis of the T-ray computed tomography reconstruction technique developed in this Thesis and its derivation is presented in Sec. 4.6.2. However, it was impossible to resist including Radon's initial inversion formula and derivation if only for its mathematical elegance and historical significance.

D.1 Derivation

Radon's original derivation provided an explicit inversion formula for the Radon transform.

$$g(\boldsymbol{\theta}, s) = \Re\{f(x)\} = \int_{x \cdot \boldsymbol{\theta} = s} f(x) dx. \quad (\text{D.1})$$

He commenced (Radon 1917, Natterer 1986) with the integral

$$\int_{|x|} f(x) \frac{1}{\sqrt{|x|^2 - q^2}} dx, \quad (\text{D.2})$$

and proceeded to evaluate the integral using two different methods. In the first method he substituted such that $x = q\boldsymbol{\theta} + s\boldsymbol{\theta}^\perp$ where $\boldsymbol{\theta}^\perp$ is the vector perpendicular to $\boldsymbol{\theta}$, $\boldsymbol{\theta} \in S$ where S is the unit circle, $s > 0$. Therefore $\frac{1}{\sqrt{|x|^2 - q^2}} dx = ds d\boldsymbol{\theta}$ and Eq. (D.2) became

$$\begin{aligned} \int_S \int_0^\infty f(q\boldsymbol{\theta} + s\boldsymbol{\theta}^\perp) ds d\boldsymbol{\theta} &= \frac{1}{2} \int_S \int_{-\infty}^{+\infty} f(q\boldsymbol{\theta} + s\boldsymbol{\theta}^\perp) ds d\boldsymbol{\theta} \\ &= \frac{1}{2} \int_S g(\boldsymbol{\theta}, q) d\boldsymbol{\theta} \\ &= \pi F_0(q), \end{aligned} \quad (\text{D.3})$$

D.1 Derivation

where $F_x(q)$ is defined as

$$F_x(q) = \frac{1}{|S|} \int_S g(\boldsymbol{\theta}, \mathbf{x} \cdot \boldsymbol{\theta} + q) d\boldsymbol{\theta}. \quad (\text{D.4})$$

Again considering Eq. (D.2) and instead substituting $\mathbf{x} = r\boldsymbol{\theta}$ we obtain

$$\int_q^\infty \int_S f(r\boldsymbol{\theta}) \frac{1}{\sqrt{r^2 - q^2}} r dr d\boldsymbol{\theta} = 2\pi \int_q^\infty \hat{f}(r) \frac{1}{\sqrt{1 - (\frac{q}{r})^2}} dr \quad (\text{D.5})$$

where

$$\hat{f}(r) = \frac{1}{2\pi} \int_S f(r\boldsymbol{\theta}) d\boldsymbol{\theta}. \quad (\text{D.6})$$

Equating Eqs. (D.3) and (D.5) we find

$$\int_q^\infty \hat{f}(r) \frac{1}{\sqrt{1 - (\frac{q}{r})^2}} dr = \frac{1}{2} F_0(q). \quad (\text{D.7})$$

This equation is an Abel integral equation. Radon solved this equation directly by computing

$$\begin{aligned} -\frac{1}{\pi} \int_0^\infty \frac{dF_0(q)}{q} &= -\frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \int_\epsilon^\infty \frac{F'_0(q)}{q} dq \\ &= \frac{1}{\pi} \lim_{\epsilon \rightarrow 0} \left\{ \frac{F_0(\epsilon)}{\epsilon} - \int_\epsilon^\infty \frac{F_0(q)}{q^2} dq \right\}, \end{aligned} \quad (\text{D.8})$$

with F_0 from Eq. (D.7) yielding

$$\begin{aligned} \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} & \left\{ \frac{1}{\epsilon} \int_\epsilon^\infty \frac{\hat{f}(r)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} dr - \int_\epsilon^\infty \int_q^\infty \frac{\hat{f}(r)}{\sqrt{1 - (\frac{q}{r})^2}} dr \frac{dq}{q^2} \right\} \\ &= \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} \left\{ \frac{1}{\epsilon} \int_\epsilon^\infty \frac{\hat{f}(r)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} dr - \int_\epsilon^\infty \hat{f}(r) \int_\epsilon^r \frac{1}{\sqrt{1 - (\frac{q}{r})^2}} \frac{dq}{q^2} dr \right\} \\ &= \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} \left\{ \frac{1}{\epsilon} \int_\epsilon^\infty \frac{\hat{f}(r)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} dr - \frac{1}{\epsilon} \int_\epsilon^\infty \hat{f}(r) \sqrt{1 - \left(\frac{\epsilon}{r}\right)^2} dr \right\} \\ &= \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} \epsilon \int_\epsilon^\infty \frac{\hat{f}(r)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} \frac{dr}{r^2} \\ &= \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} \left\{ \hat{f}(0) \epsilon \int_\epsilon^\infty \frac{1}{\sqrt{1 - (\frac{\epsilon}{r})^2}} \frac{dr}{r^2} + \epsilon \int_\epsilon^\infty \frac{\hat{f}(r) - \hat{f}(0)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} \frac{dr}{r^2} \right\} \\ &= \frac{2}{\pi} \lim_{\epsilon \rightarrow 0} \left\{ \hat{f}(0) \int_0^1 \frac{1}{\sqrt{1 - t^2}} dt + \epsilon \int_\epsilon^\infty \frac{\hat{f}(r) - \hat{f}(0)}{\sqrt{1 - (\frac{\epsilon}{r})^2}} \frac{dr}{r^2} \right\}, \end{aligned} \quad (\text{D.9})$$

here t is defined as ϵ/r .

The first integral in Eq. (D.9) is equal to $\pi/2$, and the second integral tends to 0 as $\epsilon \rightarrow 0$. Therefore

$$-\frac{1}{\pi} \int_0^\infty \frac{dF_0(q)}{q} = \hat{f}(0) = f(0). \quad (\text{D.10})$$

This may be generalised for all x giving Radon's inversion formula:

$$f(x) = -\frac{1}{\pi} \int_0^\infty \frac{dF_x(q)}{q}. \quad (\text{D.11})$$

D.2 Practical Difficulties

Radon derived an elegant solution to the idealised mathematical problem of reconstruction from projections. The major difficulties that prevented the realisation of practical tomographic systems based on Radon's original inversion formula are (Herman 1980):

- Equation (D.11) reconstructs the target using *all* its line integrals, while in practice only a finite number of projections may be measured. Given Radon's formula a subset of the projections is not sufficient to reconstruct the target uniquely, or even accurately. Using a finite number of projections results in extremely inaccurate reconstructions.
- Practical tomography systems are not capable of measuring the idealised line integral values. All practical systems include noise in the measurements, and other non-idealities such as finite sensor sizes and scattering effects further degrade the measurements. Equation (D.11) is sensitive to these error sources and this prevents accurate reconstructions from being obtained.
- Equation (D.11) is an explicit inversion formula. One of the major reasons for the strong impact of Cormack and Hounsfield's contribution was that they provided an efficient reconstruction algorithm, which permitted reconstructions to be calculated in reasonable time frames with the existing computer technology.

Appendix E

The Curse of Dimensionality

Trunk (1979) presented an elegant, yet simple example illustrating the curse of dimensionality, or the ‘peaking phenomena’. This example is adapted and summarised in this Appendix.

His example considered a d -dimensional, two-class classification problem. The prior probabilities were equal and the mean vectors for the two classes were given by

$$\begin{aligned}\mu_1 &= \left(1, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{3}}, \dots, \frac{1}{\sqrt{d}}\right), \text{ and} \\ \mu_2 &= \left(-1, -\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{3}}, \dots, -\frac{1}{\sqrt{d}}\right).\end{aligned}\tag{E.1}$$

Thus the discriminating power of each feature decreases for each successive feature. The populations are assumed to be multivariate Gaussian distributions with the d -dimensional unity matrix as the covariance for each class.

(Trunk 1979) considered two classification problems. In the first case it was assumed that the mean vector $\mu = \mu_1 = -\mu_2$ was known. The Bayes decision rule was used to classify the data and an expression for the probability of error $P_e(d)$ was derived as a function of d ,

$$P_e(d) = \int_{\theta(d)}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} dz,\tag{E.2}$$

where

$$\theta(d) = \sqrt{\sum_{i=1}^d \left(\frac{1}{i}\right)}.\tag{E.3}$$

It is simple to show that $\lim_{d \rightarrow \infty} P_e(d) = 0$. Therefore we can classify the data perfectly by arbitrarily increasing the number of features considered. However, in practice the actual mean vectors are very seldom available. So in the second case considered (Trunk 1979) assumed that μ was unknown, and instead n training vectors were available. The

maximum-likelihood estimate $\hat{\mu}$ of μ was calculated and used in the Bayes decision rule in place of μ . The probability of error of the Bayes classifier is now given by

$$P_e(n, d) = \int_{\theta(d)}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}} dz, \quad (\text{E.4})$$

where

$$\theta(d) = \frac{\sqrt{\sum_{i=1}^d \left(\frac{1}{i}\right)}}{\sqrt{\left(1 + \frac{1}{n}\right) \sum_{i=1}^d \left(\frac{1}{i}\right) + \frac{d}{n}}}. \quad (\text{E.5})$$

It can be shown that $\lim_{d \rightarrow \infty} P_e(n, d) = \frac{1}{2}$. This demonstrates that the probability of error increases to its maximum possible value of 0.5 as the number of features increases arbitrarily! This simple example clearly highlights the importance of feature extraction techniques to classification system performance. In almost all practical systems with a limited set of training data, and unknown class distributions, the number of features *must* be limited to optimise classification performance.

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Glossary

3D	Three dimensional, 2
AR	Auto-regressive, 210
CAT	Computed axial tomography, 129
CCD	Charge coupled device, 52
CSI	Contrast source inversion, 82
CT	Computed tomography, 10
CW	Continuous wave, 16
DAST	4-dimethylamino-N-methyl-4-stilbazolium-tosylate, 16
DC	Direct current, 46
DFT	Discrete Fourier transform, 57
DMEM	Dulbecco's modified Eagle's medium, 254
DNA	Deoxyribonucleic acid, 26
DSP	Digital signal processor, 46
DT	Diffraction tomography, 10
EM	Expectation maximisation, 80
EO	Electro-optic, 20
FBP	Filtered backprojection, 79
FFT	Fast Fourier transform, 46
fps	Frames per second, 56
FSEOS	Free space electro-optic sampling, 20
FTS	Fourier transform spectroscopy, 3
GaAs	Gallium arsenide, 16
HCFC	Hydrochlorofluorocarbon, 141
HCN	Hydrogen cyanide, 17
HDPE	High density polyethylene, 120
HOS	Human osteosarcoma, 253
IMPACT	Iterative maximum-likelihood polychromatic algorithm for computed tomography, 80
IR	Infrared, 2
ISP	Inverse scattering problem, 110
ITO	Indium tin oxide, 49
LIA	Lock-in amplifier, 45
LiNbO ₃	Lithium niobate, 16
LMS	Least mean square, 210
LO	Local oscillator, 20
LPC	Linear predictor coefficient, 189
MgB ₂	Magnesium diboride , 24
MGF	Modified gradient in field, 82

ML	Maximum likelihood, 79
MSE	Mean square error, 211
Nd:YAG	Neodymium-doped yttrium aluminum garnet, 17
NHB	Normal human bone, 253
NIR	Near-infrared, 46
NMR	Nuclear magnetic resonance, 35
OR	Optical rectification, 15
PCA	Photoconductive antenna, 14
RCS	Radar cross-section, 83
SAR	Synthetic aperture radar, 91
SFS	Sequential forward selection, 216
SiC	Silicon carbide, 3
SNOM	Scanning near-field optical microscopy, 38
SNR	Signal to noise ratio, 9
TDS	Time domain spectroscopy, 4
THz	Terahertz, 1
TPP	Time post pulse, 252
WFT	Windowed Fourier transform, 104
ZnTe	Zinc telluride, 16

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Résumé



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