Non-invasive detection of weapons of mass destruction using THz radiation

Matthew B. Campbell[1a] and Edwin J. Heilweil[b]
[a]SPARTA, Inc., 1911 N. Fort Myer Drive, Suite 1100, Arlington, VA, USA 22209
[b]National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD, USA 20899

ABSTRACT

The growing and immediate threat of biological and chemical weapons has placed urgency on the development of chemical and biological warfare agent (CWA/BWA) screening devices. Specifically, the ability to detect CWA/BWA prior to deployment is paramount to mitigating the threat without exposing individuals to its effects. SPARTA, Inc. and NIST are currently investigating the feasibility of using far-infrared radiation, or terahertz (THz, 1 THz = 10^{12} Hz) radiation, to non-invasively detect biological and chemical agents, explosives and drugs/narcotics inside sealed containers. Small-to-medium sized molecules (3-100 atoms) in gas, liquid and solid phases consistently exhibit identifiable spectral features in the far-IR portion of the spectrum. Many compounds associated with weapons of mass destruction are made up of molecules of this size. The THz portion of the spectrum lies between visible light and radio waves, allowing for partial transmission of 0.3-10.0 THz (30-1000 μm, 10-330 cm^{-1}) light through most common materials. Therefore, transmission measurements of THz light can potentially be used to non-invasively detect the presence of CWA/BWA, explosives and drugs in the pathway of a THz radiation beam.

Keywords: terahertz, THz, detection, weapons of mass destruction, non-invasive

1. INTRODUCTION

To assess the contribution of terahertz (THz) technologies to safeguarding individuals from weapons of mass destruction, the research team has been driven to evaluate the ability to detect and identify threat agents using THz spectroscopy. A THz spectral database has been developed that includes biological warfare agent (BWA) simulants, chemical warfare agent (CWA) simulants, explosives, pharmaceuticals, dozens of potential hoax materials as well as several types of papers and plastics used in common containers that may hold threat agents. In addition, an automated discrimination algorithm tool has been developed to identify THz spectra of bulk materials using the spectral database. By assessing the 'uniqueness' of the spectral properties of the materials of interest, and evaluating the transmission windows over the THz frequency portion of the electromagnetic spectrum for common container materials, the viability of using THz spectroscopy to non-invasively detect threats can be properly evaluated.

2. EXPERIMENTAL METHODOLOGY

Two instruments capable of collecting far-infrared spectra at room temperature (a key consideration for future applications outside the laboratory) were used to build the THz spectral database. The first is a modified Nicolet Magna 550 Fourier Transform infrared spectrometer (FT-IR) using a silicon-coated broadband beam-splitter and deuterated triglycine sulfate (DTGS) room temperature detector fitted with a high-density polyethylene window. The dry-air purged, glow bar source FT-IR has sufficient sensitivity to generate high quality spectra in the 1.5-21 THz range. All measurements made for the THz spectral database using the FT-IR were obtained at 4 cm^{-1} spectral resolution and averaging 64 interferometric scans. The second THz spectrometer is a femtosecond pulsed apparatus utilizing 120 fs pulses at 800 nm to directly generate and detect the low frequency (0.1 THz to 3.0 THz) field and spectrum (via Fourier transform) after sample transmission using ZnTe crystals [1]. Measurements with the pulsed time-domain spectrometer (TDS) are obtained at 5 cm-1 spectral resolution and averaging 50 THz pulse waveforms.

To collect transmission spectra, samples are placed directly in the beam path of the THz radiation in both instruments mentioned above. Samples are prepared in a variety of ways. For bulk solids in powder form, roughly 2 mg to 10 mg of each solid is homogenized in a mortar and pestle. The sample is thoroughly mixed with approximately 100 mg of spectro-photometric grade high-density polyethylene powder (Sigma-Aldrich, Inc.) and pressed as a pellet in a 13 mm diameter vacuum die at the lowest possible pressures (ca. 200 psi or 1.4×10^6 Pa). The 1.5 mm thick pellets have

[1] matt_campbell@rosslyn.sparta.com; phone (703) 797-3021; fax (703) 558-0045; www.sparta.com

Terahertz for Military and Security Applications, R. Jennifer Hwu, Dwight L. Woolard, Editors, Proceedings of SPIE Vol. 5070 (2003) © 2003 SPIE · 0277-786X/03/$15.00

sufficient path length to eliminate etaloning artifacts (3 cm^{-1} period) in the spectra. Sample pellets were mounted in an aluminum sample holder fixed in position with a Teflon securing ring. Spectra were converted to optical density (OD) units after ratioing raw sample transmission spectra (T_{sample}) to that of a pressed 100 mg polyethylene blank (T_{PE}) disk ($OD=-\log_{10}(T_{sample}/T_{PE})$) obtained under identical acquisition conditions. Reproducibility of THz spectral features were checked by measuring several pellets containing varying amounts of each material. The 1.5 thick polyethylene pellets restrict the spectral range available to 1.5-10 THz.

Alternatively, higher-frequency spectra (10-21 THz) of solids/powders contained in bottles can be collected by simply placing 10 mg to 20 mg of a given powder in a low-density polyethylene laboratory bottle and measuring the bottle's transmission spectrum. The spectrum of the bottle that contains the material is referenced against the spectrum of an empty bottle in the same manner as the polyethylene pellets. This technique is viable because enough residue of the powder adheres to the inner surface of the bottle to accurately observe its spectral characteristics. High transmission levels of the low-density polyethylene allows for spectral information to be collected for its contents over the entire 1.5-21 THz frequency range. We take advantage of the high transmission through low-density polyethylene to demonstrate the ability to detect aerosolized powders with THz radiation. A small chamber was built containing an agitator to disperse powders contained within the chamber. The THz beam of the FT-IR passes through the chamber (having a 15 cm path length) and a series of low spectral resolution (8 cm^{-1}) spectra are recorded as a function of time after the agitator is turned off. Each spectra is referenced against the spectrum collected after an extended aerosol settling time, to take into account the material (and inherent spectral characteristics) that collects on the input and output windows of the chamber.

3. THz SPECTROSCOPY CAPABILITIES AND LIMITATIONS

3.1 Detection of threat materials

Paramount to the practicality of using THz spectroscopy to detect and identify threat agents is the ability to identify materials by their THz spectral characteristics. Because the absorption bands observed in the spectra of the materials in the >100 items in the THz database are due to vibrational and phonon modes of the materials, they are by definition material specific. Subtle changes in the configuration of atoms in sugar molecules result in entirely different spectral features in the THz portion of the spectrum. The absorption spectra for two similar, but subtly different sugars, glucose and galactose, are shown in Figure 1, along with their molecular configuration. The significant differences in the structure in the spectra demonstrate the strong dependence of THz spectral features on crystalline atomic configuration, and thus material specificity. Therefore, THz spectroscopy can be a highly effective tool for material identification.

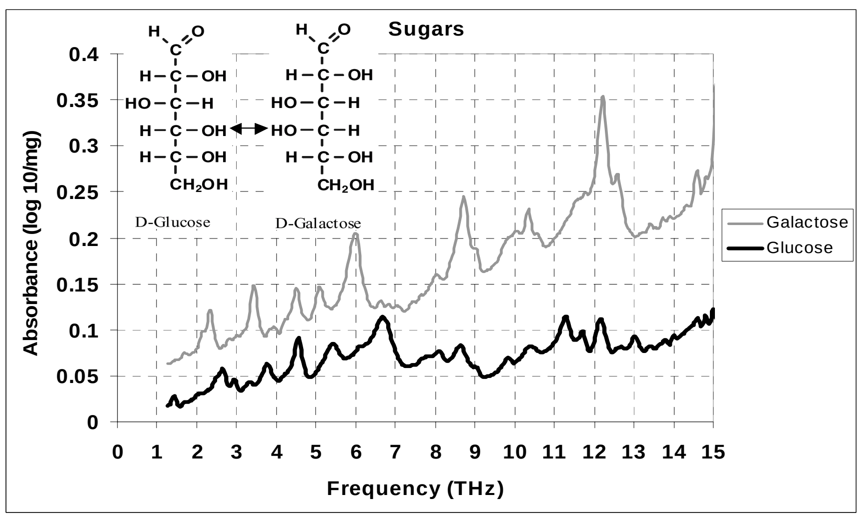

Figure 1 – Absorbance spectra for two sugars, galactose and glucose

To this end, the THz spectral database has been populated with threat materials or threat material simulants, enabling one to assess the ability to identify such materials by their THz spectral properties. Of four categories of threat materials of particular interest, 1.) biological agents, 2.) chemical agents, 3.) explosives, and 4.) drugs/narcotics, two are discussed here. In addition, the use of THz radiation to detect biological aerosols is discussed in Section 4.

Explosives Detection

The THz spectra of three explosive materials: Composition 4 (C4), pentaerythritol tetranitrite (PETN), and Semtex A, were measured over the 1.5 – 10 THz portion of the spectrum. Each of these has a unique spectral signature. The compounds found in the explosives are made of small-to-medium sized molecules, which typically have strong spectral features due to vibrational modes. Of note is the fact that Semtex A is made up of a mixture PETN and RDX, and the primary component of C4 is RDX. The THz spectrum of Semtex A contains the absorption bands found in both PETN and C4, demonstrating that in a mixture of compounds the THz spectral features continue to stand out. These distinct spectral features mean THz spectroscopy can be used to detect the presence of explosive materials in the mail or potentially in plastic hand held items.

Drug Detection

Several over-the-counter pharmaceuticals (including naproxen sodium, terfenadine, and acetaminophen) were added to the THz database. The dense spectral structure for each material indicates a high likelihood that other, illegal drugs will also have distinct THz spectra that can be used as identifiers. For example, a bottle of baby powder found in a toiletry kit can be inspected with THz radiation. The talc may be used as a cover for some illegal drug, using its strong odor to block detection by drug sniffing dogs. The THz spectrum of the mixture, however, will contain structure of all materials present. Any deviation from talc's inherent spectrum would be readily observable and provide an indication that some alternative, potentially harmful, material is present. The absorbance spectra for three pharmaceuticals included in the THz database are shown in Figure 2. The structure observed in the spectra is representative of all pharmaceutical materials in the database.

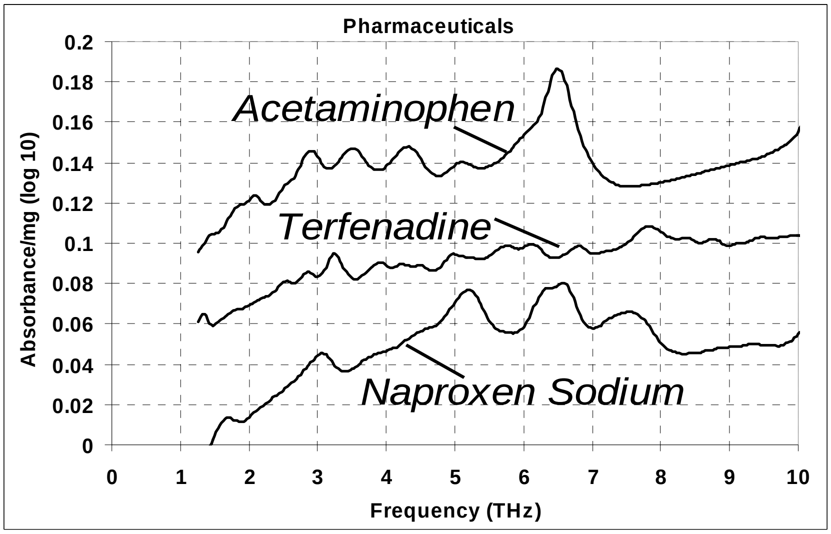

Figure 2 – Absorbance spectra for three pharmaceuticals measured with the FT-IR

3.2 Inspection capabilities

In response to the anthrax spores being delivered in the mail in the fall of 2001, the ability to inspect paper packages with THz radiation garners significant attention. All types of paper tested in this study contain sharp absorption bands at 3, 5 and 7 THz, as shown in Figure 3, which displays the absorbance spectra for three types of paper and cellulose. These bands are attributed to the presence of cellulose in the paper because it has the same spectral features. The relative uniformity between paper types implies the contribution of paper can effectively be removed from a spectrum, leaving the spectral features of any additional material. The spectra of 10 types of paper and cellulose are included in the THz spectral database.

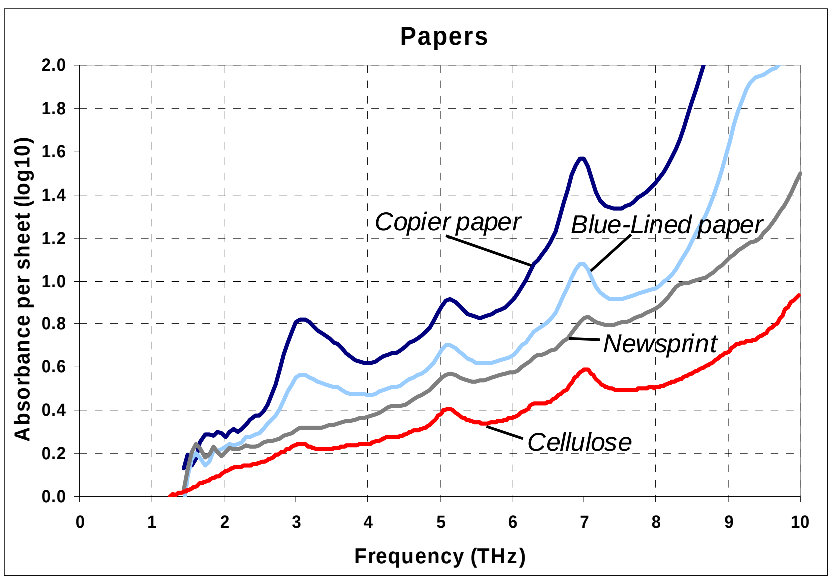

Figure 3 – Absorption spectra of different types of paper and cellulose

3.3 Automated detection and identification of materials

To identify a material, its spectrum is entered into a THz spectroscopic Automated Discrimination Algorithm (ADA) Tool, which produces a sorted list of all the materials in the THz database ranked from closest match to worst match with regards to the entered spectrum. The compilation of the output for each spectrum in the test set is used to evaluate the true positive and false positive rates. An example of the output of the ADA Tool is shown in Figure 4. The ADA Tool uses several spectral comparison methods to compare the spectrum of an unknown/unidentified material to each material in the database. The rank-ordered list also provides the relative 'closeness' of the spectrum of the unknown material to the best match and to the other materials in the database, which can be used to assess the confidence level in the match. For example, if the top 5 materials in the ranked list all have about the same score, there is a lower probability that a correct match has been made.

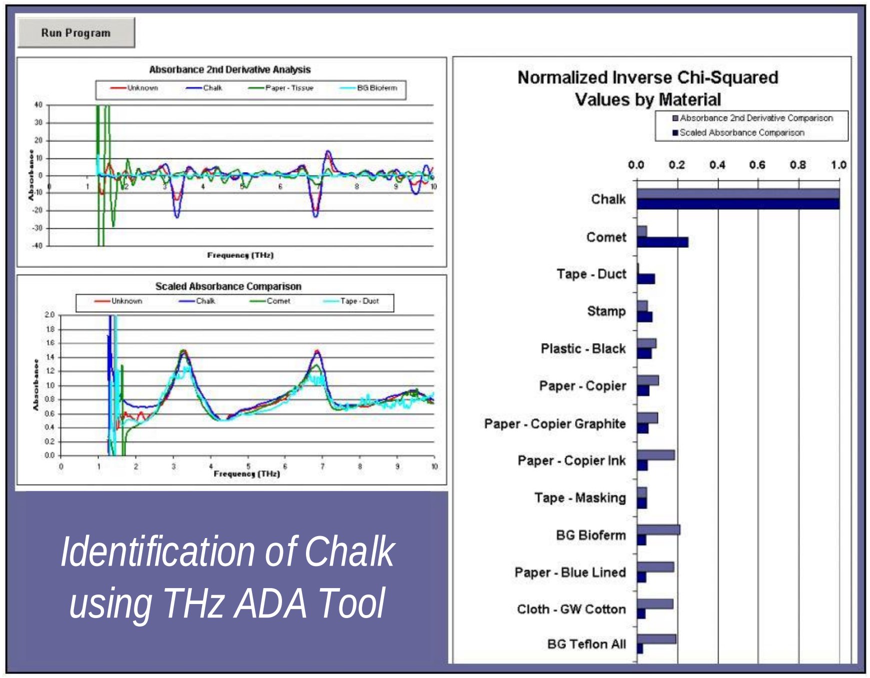

Figure 4 - Screenshot of the ADA Tool output demonstrating the ability to accurately identify materials housed in sealed containers by only considering the THz transmission spectrum of the container.

3.4 Limitations

When considering THz technologies for detection of threats in container applications, the inherent limitations and operational risks must be considered. The primary limitation of THz spectroscopy is radiation throughput.

The equipment used in the experiments performed for this effort generate and detect THz radiation with tabletop instrumentation that operates at room temperature, two requirements for devices to be implemented in an environment outside the laboratory. These devices (the pulsed TDS system and FT-IR with DTGS detector) typically have low far-infrared power (less than a micro-Watt at a given frequency) and have limited sensitivity, especially the FT-IR. As a result, the overall thickness limits one's ability to inspect a container using these approaches. We find that attenuation of THz radiation in paper limits transmission measurements to <5 THz when performing inspections through 2 or more sheets of paper using the standard FT-IR glow bar and room temperature DTGS detector.

There are two additional limitations to THz transmission spectroscopy. First, THz radiation does not transmit through metal. Second, glass only transmits THz radiation at frequencies lower than 1 THz, greatly restricting the spectral information that can be collected through a glass container. This limitation is potentially mitigated with other techniques, such as Raman spectroscopy.

4. APPLICATIONS OF THz SPECTROSCOPY

Given the capabilities and limitations discussed above, THz spectroscopy has the potential to be used in several areas for rapid and efficient detection and identification of WMD. Two of these areas are considered below. The first is rapid screening of the mail for the presence of some foreign material contained in an envelope. Detection of such materials in the mail system may significantly reduce the strain on the mail system, which treats all articles of mail as a threat and sends them to an electron beam irradiation facility. Similarly, rapid detection of threat materials can potentially safeguard employees of a mail sorting facility and enable rapid forensic processing for law enforcement officials. The second application discussed below is biological aerosol detection. Current aerosol systems are susceptible to high false alarm rates and THz spectroscopy may enhance overall point and standoff detection capabilities.

Mail Screening

A second operational scenario in which current THz technologies are appropriate is rapid screening of the mail for foreign material. The beam from a high-powered, continuous wave (CW) THz laser can possibly be split into several beams to monitor the relative transmission through different regions of an envelope to detect unexpected in-homogeneities in the envelope. If an envelope simply carries only folded paper the transmission through different portions of the envelope will be uniform. Alternatively, if an envelope contains some foreign material, such as an unidentified powder, it is expected that the powder may settle on one side of the envelope inducing significant variations in the transmission of THz radiation through different portions of the envelope.

A potential THz screener could a high-powered THz laser that operates at a single frequency and generates ~100 mWatts of power (six orders of magnitude greater power at a given frequency than the TDS or FT-IR systems). The high power allows for transmission measurements through standard envelopes (those associated with 1st class mail delivery) and perhaps through cardboard packages. An array of DTGS detectors configured to form a low resolution THz imager could be used to inspect each envelope as it passes by the screener. Any large disparity between, or universal attenuation of, the transmission levels to the detectors would indicate something atypical or unexpected was contained in an envelope. That envelope can be filtered to a separate area of the mail sorting facility for either further inspection or irradiation by an electron beam. The rest of the items of mail, the ones that appear uniform, would continue through the mail system because they are highly unlikely to contain some potentially harmful material.

Aerosol Detection

We have explored the possibility of directly detecting spore-containing aerosols by THz absorption spectroscopy. We recently built an enclosed sampling chamber capable of stirring and aerosolizing powders within the THz Nicolet FT-IR bench. Samples of pure silica and BT spores supported on silica/alumina were investigated. As shown in Figure 5, we observed strong spectral signatures in the 10 to 20 THz spectral range that decay as a function of time after the stirrer is

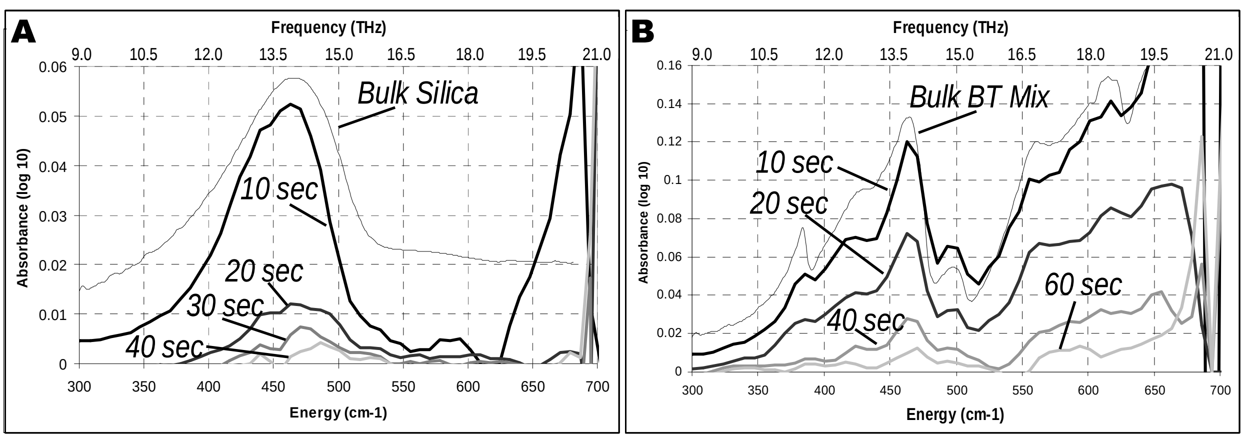

Figure 5 – Direct detection and identification of aerosols with an FT-IR configured for far-infrared spectroscopy. Absorbance spectra measured through a plastic (LDPE) container containing A.) Cab-O-Sil ™ silica and B.) a mixture of BT spores, alumina and silica at different times after an agitator was turned off are shown. As time passes, less material remains suspended in air and a decrease in total absorption of THz radiation is observed. In addition, readily available spectral information allows for identification of each aerosol, as shown by the spectra for silica and the BT spore mixture in bulk form.

stopped. These materials are readily identified by their distinctly different THz spectral features. The data also show that as sample particulates settle to the bottom of the chamber, diminishing amounts of material is observed through transparent polyethylene windows at the top where the THz beam traverses the chamber (15 cm path length). It should be pointed out that we were able to measure air-borne material THz spectral features in the absence of visible scatter within the chamber. The FT-IR typically has sufficient sensitivity to measure identifying spectral features of materials for bulk samples of ~200 micrograms.

5. SUMMARY

Pre-release detection of threats is critical for safeguarding individuals from terrorist attacks and enabling law enforcement officials to quickly track down the sources of such threats. Preliminary studies strongly indicate THz technologies may provide the capability of non-invasive, non-destructive, material specific detection of threats in bulk and aerosol form. As higher-powered THz sources and more sensitive THz sensors become available, robust THz screening systems are likely to become viable.

ACKNOWLEDGEMENTS

The authors would like to thank Ms. Heather McCarthy of SPARTA, Inc. for development work of the THz spectral Automated Discrimination Algorithm Tool and Drs. Larry Iwaki, Timothy Korter and Matthew Beard of NIST for continued support with pulsed TDS system.

REFERENCES

[1] P. Y. Han and X.-C. Zhang, Appl. Phys. Lett., 73 (1998) 3049.