Guided Wave THz Spectroscopy of Explosive Materials

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Abstract

One of the important applications of THz time-domain spectroscopy (TDS) is the detection of explosive materials through identification of vibrational fingerprint spectra. Most recent THz spectroscopic measurements have been made using pellet samples, where disorder effects contribute to line broadening, which results in the merging of individual resonances into relatively broad absorption features. To address this issue, we used the technique of parallel plate waveguide (PPWG) THz-TDS to achieve sensitive characterization of three explosive materials: TNT, RDX, and HMX. The measurement method for PPWG THz-TDS used well-established ultrafast optoelectronic techniques to generate and detect sub-picosecond THz pulses. All materials were characterized as powder layers in 112 μm gaps in metal PPWG. To illustrate the PPWG THz-TDS method, we described our measurement by comparing the vibrational spectra of the materials, TNT, RDX, and HMX, applied as thin powder layers to a PPWG, or in conventional sample cell form, where all materials were placed in Teflon sample cells. The thin layer mass was estimated to be about 700 μg, whereas the mass in the sample cell was ~100 mg. In a laboratory environment, the absorption coefficient of an explosive material is essentially based on the mass of the material, which is given as: α(ω) = [ln(I₀(ω)/I(ω))] / m.

In this paper, we show spectra of 3 different explosives from 0.2 to 2.4 THz measured using the PPWG THz-TDS.

Key words: Terahertz, Waveguide, Spectroscopy, TNT, RDX, HMX.

I. Introduction

The Terahertz (THz) range is typically defined as the frequency range from 0.1 to 10 THz. Wavelength of THz is 3 mm ~ 30 μm. Due to the difficulties in generating and detecting THz, the THz range is viewed as one of the most inaccessible. The recent development of nanomaterial technology and ultrafine processes has allowed the advent of new THz sources. The commercialization of techniques for ultrashort femtosecond laser pulses has also accelerated the development of techniques for generation and detection of THz [1].

At present, THz applications are being intensively studied in various fields such as new materials, medicine, biology, security, defense, environment, space, and communication [2]. Terahertz time domain spectroscopy (THz-TDS) is one technology that is used for analysis of materials. This technology can be used to obtain the phase information of materials directly through the vibration spectrum, conformational change, and the E-field measurement of THz pulse. Complex refractive index, complex dielectric properties, and complex conductivity can also be obtained using these techniques. One important application of THz-TDS is the detection of explosive and prohibited materials through identification of vibrational fingerprint spectra [3~4].

During the past ten years, THz waveguides, which could be applied in various fields including THz communication, have been reported in terms of a rectangular waveguide [5], a circular waveguide [6], a fiber [7], a single wire [8], a coaxial cable [9], planar transmission lines [10], and parallel plate waveguides [11]. Because these THz waveguides can focus the electromagnetic energy on a microsize structure, the use of THz-TDS waveguides allows analysis of traces of powder or thin films that previous THz-TDS was unable to access. Compared with other waveguides, parallel plate waveguides (PPWG) show a particularly rare dispersion of group velocity. When the polarization of the incident electric field is perpendicular to the metal plane of a PPWG, a single TM mode propagation is possible. In addition, because the cutoff frequency does not exist in a single TM mode, PPWG is more suitable for application in spectroscopy than any other type of waveguide [12~13].

In the present paper, we report a unique THz-TDS system based on a PPWG. This system has sufficient sensitivity to detect prohibited materials and explosives. The ability to detect these materials at security checkpoints for airports, seaports, subways, and other major
public facilities has become a serious security issue. We confirmed that our THz-TDS system was useful for detecting small amounts of explosive powders (TNT, RDX, HMX). We also expect that our THz-TDS system can be utilized for the analysis of trace amounts of biochemical and other materials.

II. Experimental Setup

Fig. 1 shows the schematic diagram of the complete THz-TDS system. This system consists of a Ti: Sapphire femtosecond laser, optical time delay devices, THz generators and detectors of the photoconductive antenna system, parabolic mirrors, a lock-in amplifier, and an optical chopper [14~15].

A femtosecond laser beam is divided by a beam splitter into a pump beam and a probe beam. The pump beam is directed at the transmitter chip (Tx) to generate a THz wave. The probe beam is directed at the receiver chip (Rx) to detect the THz wave. With this structure, a time delay exists between the two beams due to the length of the beam path. To avoid this delay, we used a delay line, as shown in Fig. 1. The Tx and Rx chips were patterned using low-temperature grown GaAs. Silicon lenses were attached to the Tx and Rx chips for proper radiation and focusing of the THz wave. THz waveform can be obtained by measuring an output signal from the detect antenna using a lock-in amplifier.

Fig. 2 shows the designed Teflon sample cell and PPWG to investigate the spectroscopy of explosive materials (TNT, RDX, HMX). Because Teflon in the THz band has very small refractive index and very low absorption characteristics, it can be called an ideal material for the spectroscopy of explosive materials. The Teflon sample cell has the dimension of 30×30 mm and the thickness of 15 mm. This cell has a room with the dimension of 15×15 mm and the thickness of 1 mm in order to put explosives in it. Fig. 2(b) shows the PPWG with the dimension of 30×38 mm and the thickness of 10 mm, respectively. Silicon lenses on which THz wave can be focused have the dimension of 15×9.1 mm and the height of 7.07 mm.

III. Measurements

Fig. 3(a) shows the THz-TDS system using the Teflon sample cell containing explosive materials (TNT, RDX, HMX). The Teflon sample cell was located on the center path of the beam, between two parabolic mirrors. We measured the reference pulse on the cell without explosives and the signal pulse with explosives in this system.

Fig. 3(b) shows the THz-TDS system using the PPWG containing the same explosive materials. The PPWG was also located on the center path of the beam, between the same mirrors. We obtained the reference pulse and the signal pulse by mounting explosives on the bottom part of the PPWG, as shown in Fig. 3(c). No explosives were added to the upper part of the PPWG, to allow measurement of the reference pulse.

We can obtain the electric field of the THz pulse transmitted to the samples (the Teflon sample cell or PPWG) in the time and frequency domains using the fast fourier transformation (FFT).

In a laboratory environment, the absorption coefficient of an explosive material is essentially based on the mass of the material, which is: \( \alpha(\omega) = \frac{\ln(I_R(\omega)/I_S(\omega))}{m} \). Here, \( I_R \) is the reference signal power of the THz wave, \( I_S \) is the THz power measured after the transmission through the sample, and \( m \) is the mass of the explosive material [1]. All materials are characterized as powder layers in the 112 μm gap of the metal parallel plate [16~17]. The thin layer mass in the PPWG was estimated to be about 700 μg, whereas the mass in the Teflon sample cell was \(~\)100 mg.
IV. Results

Fig. 4(a) shows the signal and the reference pulses for TNT measured through the teflon sample cell. The THz pulse at 29~31.2 ps was the reference pulse without TNT and the THz pulse at 29.8~32 ps was the signal pulse with TNT. The difference of 0.8 ps indicates the time delay due to the refractive index of TNT. The amplitude of the TNT signal pulse also becomes 3 times smaller than that of the reference pulse. The full width half maximum (FWHM) of the signal pulse and the reference pulse was 0.4 ps. We could calculate electrical and optical properties such as absorption of materials, refractive index, and electrical conductivity by measuring the phase variation and amplitude variation of the THz wave. Fig. 4(b) shows the frequency spectra for the reference and signal pulses. These results can be obtained by FFT from Fig. 4(a). As shown in Fig. 4(b), the range of frequency for the reference pulse was 0~3.5 THz and that for the signal pulse was 0~2.5 THz. The amplitude of frequency spectrum for the signal pulse reduces to 50 %, compared with that for the reference pulse. This possibly can be attributed to energy absorption by TNT. Fig. 4(c) presents the intrinsic absorption spectrum calculated by $a(w) = [\ln(I_s(w)/I_r(w))] / m$. Weak peaks are present at about 1.0 THz, 1.26
Fig. 5. (a) The measured TNT THz pulse in time domain through the PPWG with 112 μm plate separation. The reference pulse (solid) and signal pulse (dot). (b) The calculated TNT THz pulse in the frequency domain by FFT. (c) Calculated absorption coefficient of TNT.

THz, and 1.6 THz.

Fig. 5(a) shows the signal and reference pulses for TNT measured through the PPWG. As shown in Fig. 5(a), the amplitude of the signal pulse was 3 times smaller than that of the reference pulse. This can also be attributed to energy absorption by TNT. The THz pulse at 36~38.2 ps was the reference pulse and the THz pulse at 36.8~39.4 ps was the signal pulse. Fig. 5(b) shows the frequency range for TNT by the PPWG. The frequency spectrum of the reference pulse was 0~3 THz and that of the signal pulse was 0~2.5 THz. We can also observe some energy absorptions by TNT from the frequency spectrum. Fig. 5(c) presents the intrinsic absorption spectrum by the PPWG for TNT. Sharp peaks at about 1.0 THz, 1.2 THz, 1.3 THz, and 1.66 THz were observed. We could also readily confirm other clear peaks at 1.2 THz and 1.3 THz compared with results using the Teflon sample cell as shown in Fig. 4(c). The results of Fig. 5(c) were based on 140 times smaller mass (700 μg) of explosives than that (100 mg) in the Teflon sample cell. This means that THz-TDS using the PPWG was more sensitive than THz-TDS using the Teflon sample cell.

Fig. 6(a) shows the signal and reference pulses for RDX measured through the Teflon sample cell. The THz pulse at 10.6~13.2 ps was the reference pulse without RDX and the THz pulse at 12.4~15.6 ps was the signal pulse with RDX. The difference of 1.8 ps indicates the time delay due to the refractive index of RDX. The amplitude of the signal pulse for RDX was also 7 times smaller than that of the reference pulse. The full width half maximum (FWHM) of the reference pulse was 0.3 ps and that for the signal pulse was 0.5 ps. Fig. 6(b) shows the frequency spectra for the reference and signal pulses. These results can be obtained by FFT from Fig. 6(a). As shown in Fig. 6(b), the frequency spectrum for the reference pulse was 0~3 THz and that for the signal pulse was 0~2 THz. The amplitude of the frequency spectrum for the signal pulse reduces to 50% of that of the reference pulse. We think that this can be attributed to the energy absorption by RDX. Fig. 6(c) presents the intrinsic absorption spectrum. Weak peaks are seen at about 0.82 THz, 1.05 THz, 1.5 THz, and 1.96 THz.

Fig. 7(a) shows the signal and reference pulses for RDX measured through PPWG. As shown in Fig. 7(a), the amplitude of the signal pulse was 3 times smaller than that of the reference pulse. This can also be attributed to the energy absorption by RDX. The THz pulse at 35~36.9 ps was the reference pulse and the THz pulse at 34~41 ps was the signal pulse. Fig. 7(b) shows the frequency spectrum for RDX by the PPWG. The frequency range of the reference pulse was 0~3.5 THz and that of the signal pulse was 0~2.5 THz. Other energy absorptions for RDX are seen in the frequency spectrum. Fig. 7(c) presents the intrinsic absorption spectrum by the PPWG for RDX. Sharp peaks at about 0.82 THz, 1.05 THz, 1.36 THz, 1.56 THz, and 1.96 THz were observed. We could also readily confirm other clear peaks at 1.36 THz and 1.56 THz compared with results from the Teflon sample cell, as shown in Fig. 7(c). The results shown in Fig. 7(c) were based
Fig. 6. (a) The measured RDX THz pulse in time domain through the Teflon sample cell. The reference pulse (solid) and signal pulse (dot). (b) The calculated RDX THz pulse in the frequency domain by FFT. (c) Calculated absorption coefficient of RDX.

on 140 times smaller mass (700 μg) of explosives than that (100 mg) of the explosives in the Teflon sample cell.

Fig. 8(a) shows the signal and reference pulses for HMX measured through the Teflon sample cell. The THz pulse at 28.7~31 ps was the reference pulse without HMX and the THz pulse at 29.7~32 ps was the signal pulse with HMX. The difference of 1 ps indicates the time delay due to the refractive index of HMX. The amplitude of the signal pulse for HMX was also 3 times smaller than that of the reference pulse. The full width half maximum (FWHM) of the reference pulse was 0.3 ps and that for the signal pulse was 0.5 ps. Fig. 8(b) shows the frequency spectra for the reference and signal pulses. These results can be obtained by FFT from Fig. 8(a). As shown in Fig. 8(b), the frequency spectrum for the reference pulse was 0~3 THz and that for the signal pulse was 0~2.3 THz. The amplitude of the fre-
Fig. 8. (a) The measured HMX THz pulse in time domain through the Teflon sample cell. The reference pulse (solid) and signal pulse (dot). (b) The calculated HMX THz pulse in the frequency domain by FFT. (c) Calculated absorption coefficient of HMX.

Fig. 9. (a) The measured HMX THz pulse in time domain through the PPWG with 112 μm plate separation. The reference pulse (solid) and signal pulse (dot). (b) The calculated HMX THz pulse in the frequency domain by FFT. (c) Calculated absorption coefficient of HMX.

The frequency spectrum for the signal pulse drops to 50% of that of the reference pulse. We think that this can be attributed to the intrinsic absorption spectrum, showing a weak peak at about 1.78 THz.

Fig. 9(a) shows the signal and reference pulses for HMX measured through the PPWG. As shown in Fig. 9(a), the amplitude of the signal pulse was 2 times smaller than that of the reference pulse. This can also be attributed to the energy absorption by HMX. The THz pulse at 36.8 ~ 39.8 ps was the reference pulse and the THz pulse at 38 ~ 41 ps was the signal pulse. Fig. 9(b) shows the frequency spectrum for HMX by the PPWG. The frequency spectrum of the reference pulse was 0 ~ 4 THz and that of the signal pulse was 0 ~ 2.5 THz. Energy absorptions peaks can also be seen for HMX from the frequency spectrum. Fig. 9(c) presents the intrinsic absorption spectrum by the PPWG for HMX, showing a sharp peak at about 1.78 THz was observed. The results shown in Fig. 9(c) were based on 140 times
smaller mass (700 $\mu$g) of explosives than that (100 mg) of explosives in the Teflon sample cell. Based on the measurements of 3 explosive materials, we can easily verify that THz-TDS using the PPWG was superior to THz-TDS using the Teflon sample cell.

V. Conclusion

In this paper, we characterized the fingerprint of 3 explosive materials (TNT, RDX, HMX) using THz-TDS with a Teflon sample cell and PPWG. We identified the absorption spectra for 3 materials previously studied by several research groups. We also observed the same absorption spectra through THz-TDS with the PPWG. However, we were able to obtain clear results with high resolution, compared with THZ-TDS with a Teflon sample cell. We were also able to obtain additional and more accurate information for the intrinsic absorption spectra, even though we used 140 times smaller mass of explosives than that used for explosives for THz-TDS with a Teflon sample cell.

We expected that our system with the PPWG would readily detect various explosive materials and could also analyze traces of biochemical and other materials. Homeland security could further develop our system for the detection, for example, of mines and other explosives and for use in searches for prohibited materials. In addition, if we construct a database for the fingerprints of various prohibited materials as our next step, we can provide public facilities such as airport, seaport, subway and post office with fingerprints for various dangerous materials.

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