

THz spectroscopy of explosive-related simulants and oxidizers

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Abstract. In this paper we report on measurement of spectra of commonly applied explosives, some materials which can be used for manufacture of explosive and THz simulants of explosives in transmission mode. Substances were prepared as pellets, and the measurements were performed using the Time Domain Spectroscopy system in the range 0.1–3.0 THz

Key words: THz spectroscopy, explosive-related simulants.

1. Introduction

Strong interest in terahertz radiation (0.1–10 THz) especially in the security industry is connected with its unique features. Terahertz waves penetrate many materials apart from metals or polar mediums (like water). Therefore, terahertz radiation can scan through packing, clothes, shoes, bags and is suitable for screening baggage and primarily for looking for materials hidden on human body under coverings. Such advantages are of great importance for security and defense related applications [1, 2].

Chemical compounds of dangerous materials have specific absorption and reflection spectra in terahertz range, which enables to identify them. So, many explosives (e.g., Hexogen, Penthrate, Trinitrotoluene, Octogen) have characteristic transmission features in the THz range that could be distinguishable from other common materials like clothes, human skin or metal materials. Basing on our initial research and literature [1, 2] we focused only on materials which have some characteristic features in THz range. Unfortunately, transmission spectra of some dangerous materials like Ammonium Nitrate-based explosives (Saletrol, Ammonal) or Picric Acid have broad Terahertz absorption profile with no sharp spectral features.

Development of terahertz technology for security is somewhat limited because of the danger associated with the production, storage and measurements of explosives which require special safety precautions. Due to limited number of THz laboratories certified for explosive handling it is necessary to find simulants, which are easy to use, and have characteristic fingerprints similar to hazardous materials, but are readily available and do not pose a danger to persons engaged in research with them.

In this paper we report on measurements absorption spectra of Hexogen (RDX), Penthrate (PETN) and Octogen (HMX) compared with absorption spectra of their simulants in the range 0.1–3.0 THz. The obtained characteristics can be used to select safe materials with characteristics similar to the explosives. This will enable the development of terahertz technology for security research centers that do not have direct

access to hazardous materials. In addition to the explosives and their simulants we also measured some oxidizers which are not necessarily combustible, but may, generally by yielding oxygen, cause or contribute to the combustion of other material.

Spectra of the above mentioned materials were measured by many groups but their results can differ due to different preparation procedure, age and type of explosive, preparation technique of pellets, different measurement technique and conditions (temperature, humidity etc.). So, we decided to measure the spectra independently to create own data base of compounds with known measurement conditions.

Spectral measurement of materials in THz range can be performed by Time Domain Spectroscopy (TDS) [1, 2, 6, 7], Photomixer setup [3], Fourier Transform Spectroscopy [1] as well as Quantum Cascade Laser-based system [4]. For our investigations we choose TDS system due to its high sensitivity and repeatability in 0.1–3.0 THz range. The considered materials have also spectroscopic features in the range above 3 THz, but due to high attenuation of commonly used package materials (like paper or clothes) in this range, what makes a detection of hidden materials problematic, as well as measurement possibilities of our system, we limited our research only to 0.1–3.0 THz range.

2. Sample preparation

Sample preparation is a very important factor to obtain a reliable spectra. Attenuation of pure explosives is too high to obtain reliable measurements in THz range, so in order to prepare samples 10% of explosives was mixed with 90% of Teflon (PTFE) to obtain 1 g of a mixture. Next, it was mixed with ethanol and mashed in a mortar to get even mixture and dried through 30 minutes. Afterwards, the powder was weighted to obtain 400 mg, loaded to a form and pressed with 2 tons of pressure. As a result, a pellet with diameter of 13 mm and thickness of about 1.4 mm was obtained. As a reference, a pellet made of pure Teflon with the same dimensions was prepared. A similar method was applied to simulants, but

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instead of explosives Sugar, Tartaric Acid and Aminobenzoic Acid were used.

3. Time Domain Spectrometry – transmission configuration

For Time Domain Spectroscopy measurement, Teraview TPS 3000 unit in transmission configuration was used. Time Domain Spectroscopy is a commonly used technique in THz range and is described in detailed in many books and papers, e.g. [1, 2, 6, 7].

In Time Domain Spectroscopy (TDS) we measured spectra of the material sample (T_M) and the reference sample (T_R). The transmission spectra of the explosives, simulants and oxidizers can be presented as absorbance (A), which is defined as:

$$A = -\log_{10} \left(\frac{T_M}{T_R} \right). \quad (1)$$

However, absorbance depends on sample thickness and cannot be used for spectra comparison of two samples with different thicknesses. So, absorbance is commonly transformed to absorption coefficient (α), which is defined as:

$$\alpha = -\frac{1}{l} \ln \left(\frac{T_M}{T_R} \right), \quad (2)$$

where l is the effective thickness of the pure explosive material in the sample. We assumed that thickness of a pure explosive, which is evenly distributed inside the sample, can be converted to the effective thickness of the explosive by the formula:

$$l = \frac{m}{\rho} \frac{4}{\pi D^2}, \quad (3)$$

where ρ is the density of the explosive material, m is the weight of the sample and D is the diameter of the sample.

The main parameters of the transmission configuration (Fig. 1) of the systems are: spectral range 0.1–3.0 THz, signal-to-noise better than 4000:1, dynamic range higher than 3 OD in the range 2 cm^{-1} to 100 cm^{-1} , spectral resolution 0.06 THz and rapid scan mode with 30 scans/second. The pellets were placed in the middle of the distance between the emitter and detector, perpendicularly to the incident THz beam. The chamber was purged with dry air to eliminate water vapor [5].

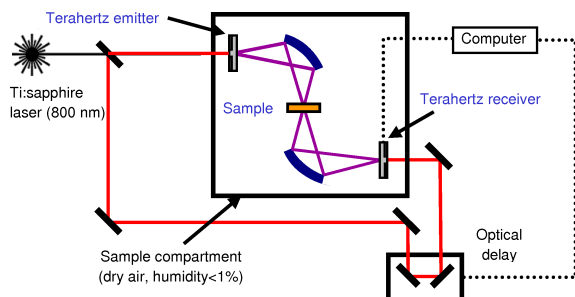


Fig. 1. Teraview Time Domain Spectroscopy – transmission configuration after Ref. [5]

4. Results and discussion

Figures 2–5 present transmission spectra of commonly used explosives compared with simulants which, unlike the explosives could be safely manufactured and used for measurements. Figure 2 presents transmission spectra of PETN compared with its simulant (Sugar). It is clearly seen that two main peaks in PETN spectra have their counterpart in sugar spectra. These peaks are shifted by about 0.2 THz, but both characteristics are similar in terms of shape. It can be concluded that Sugar is a good simulant of PETN.

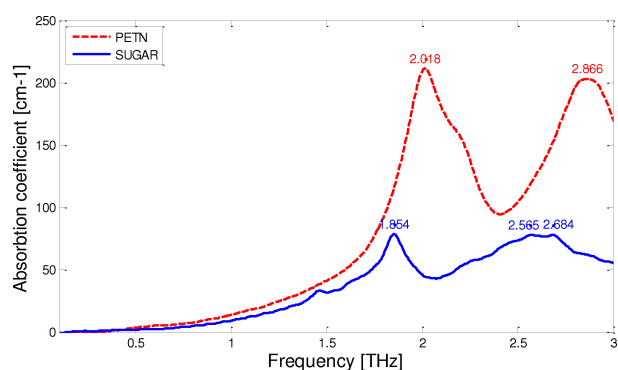


Fig. 2. Transmission spectrum of PETN and its simulant SUGAR

A similar situation can be observed in Fig. 3 which shows the comparison of RDX and its simulant (Tartaric Acid). In this case, simulant peaks are also shifted, but generally characteristics are very similar in shape.

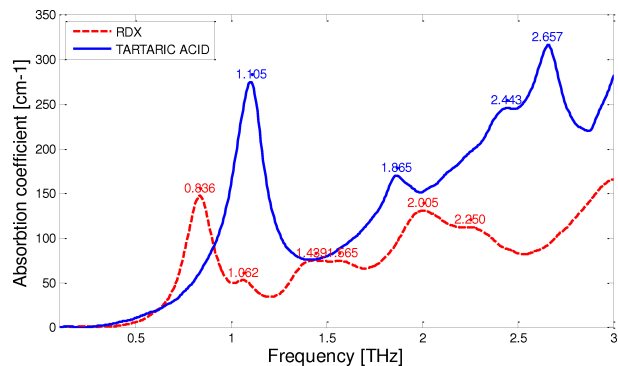


Fig. 3. Transmission spectrum of RDX and its simulant TARTARIC ACID

Unfortunately, not every dangerous material has its own simulant in THz range. For these materials, it is possible to simulate the single peaks. Figure 4 shows HMX and Aminobenzoic Acid which is not an exact simulant, but some peaks in its characteristics are similar to those occurring in the characteristics of HMX.

Not only pure explosives are dangerous. Detection of materials such as oxidizers, described in introduction, is also necessary. The primary hazard associated with this class of compounds lies in their ability to act as an oxygen source, and thus to readily stimulate the combustion of materials. The question is whether they have characteristic peaks in the THz frequency range. Figure 5 shows that such oxidizers as

KNO_3 and KClO_3 have such peaks in the THz band. Peaks obtained by us during the measurements are very similar to those reported in other publications [2].

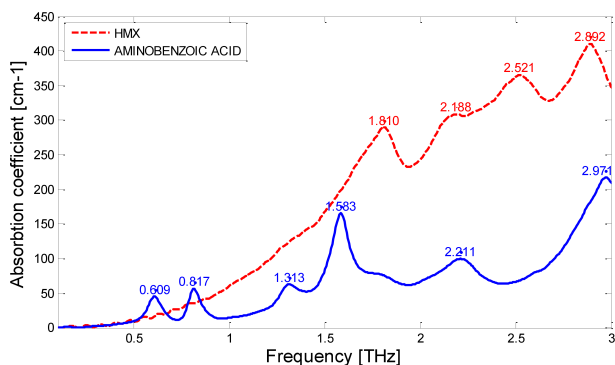


Fig. 4. Transmission spectrum of HMX and its simulant AMINOBEZOIC ACID

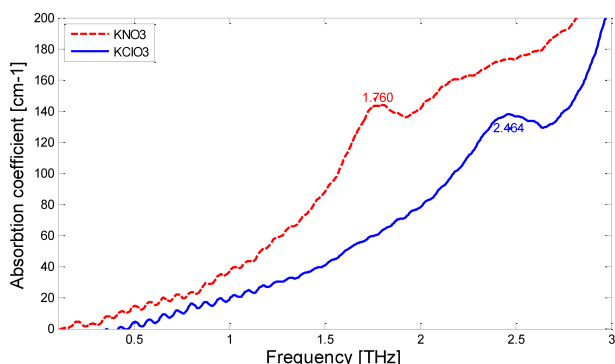


Fig. 5. Transmission spectrum of oxidizers (KNO_3 and KClO_3)

5. Summary

Spectra of some pure explosives (PETN, RDX, HMX) and their simulants (Sugar, Tartaric Acid and Aminobenzoic Acid) were measured in transmission mode in Teraview TPS 300 TDS system. Peaks in absorbances of all dangerous substances

find their equivalents in characteristics of their simulants, the shapes are also very similar. Results obtained in the measurements of oxidizers show that THz measurements can be used for detection not only explosives, but also the accompanying them dangerous materials. However, due to relatively high attenuation of the presented dangerous materials, transmission spectroscopy can be only used for screening of small packages, like mails, to find small amounts of powders.

In real applications, for scanning of bigger packages or people reflection spectroscopy should be applied. Unfortunately, due to small reflection of dangerous materials and strong dependence on surface quality, this kind of measurement requires more sensitive arrangements and careful signal processing to obtain reliable results.

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