# Extension of the *p*-Spectrum Method to the Higher Frequencies

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The *p*-spectrum method is a time domain spectroscopy-based technique for reflection analysis of materials (including explosives) that takes into account only part of the reflected signal, which is next analyzed via the Fourier transform. The method is limited to the frequencies of about 1.8 THz due to the pulse properties of our time domain spectroscopy setup. In this paper we theoretically prove that application of a shorter pulse can increase this frequency range up to 2.2 THz, that enables analysis of penthrite and octogen, two important explosives.

## 1. Introduction

The stand-off detection of many substances, including explosive materials, has been focusing attention for over three decades. Some commonly used explosive materials, like hexogen (RDX), octogen (HMX), and penthrite (PETN) have very characteristic spectral transmission and reflection features in the THz range of radiation (0.1–3.0 THz) [1–6]. Only reflection geometry seems to be applicable for a remote detection of explosive due to their high absorption in the THz range. Unfortunately, there are many factors that influence this kind of measurement: surface morphology, size of particles inside a sample, coverings, and geometry of the detecting system [7–9].

Time domain spectroscopy (TDS) is a commonly used technique for spectral characterization of materials both in transmission and reflection configurations [1–9]. It is based on the analysis of a very short, usually less than 1 ps long, pulse of electromagnetic radiation, which has very broad useful bandwidth, usually 0.1–3.0 THz, and high sensitivity (up to 70 dB).

In the reflection configuration, the reflectance can be experimentally determined by dividing the power spectrum from the sample by the power spectrum from a gold reference mirror, measured in identical way. The peaks in the absorbance profiles of the materials are associated with characteristic features (slopes) visible in the reflectance diagram that can be explained using dispersion at a resonance in the Lorentzian harmonic oscillator model. Reflectance of most materials is usually below 0.15, while the slope amplitude is normally in the range of 0.03–0.12 depending on the material and the incident angle [10]. That is why the identification of the materials is demanding, especially taking into account small contrast of these slopes.

Therefore, the *p*-spectrum method for extraction of the characteristic features of these materials was proposed

previously [11]. Briefly, the method takes into account only part of the pulse reflected from a sample, which is next analyzed in the frequency domain by the Fourier transform. The obtained spectrum has very distinctive peaks, which correspond to main peaks measured in the transmission configuration and make a reliable identification possible. A spectrum characteristic of the TDS pulse decreases with frequency and limits the application of the method to the frequencies up to 1.8 THz. Therefore, first absorption peak of RDX at 0.84 THz can be easily investigated, while peaks of HMX and PETN, which are situated at 1.81 THz and 2.02 THz, respectively, are hard or impossible to identify [11].

This limitation is due to the fact that a TDS setup, which was used for the measurements, is based on the photoconductive antennae that can generate the pulse with the full width at half maximum (FWHM) of about 0.4 ps. Its power spectrum has its maximum at 0.5 THz and decreases to about −25 dB at 2 THz. In this paper we theoretically prove that this drawback can be overcome if the setup with wider bandwidth obtained by means of a shorter pulse, lasting about 0.1 ps, is used. Such pulses can be generated using a laser-induced gas plasma technique [12] or TDS setups with organic crystals (DAST, DSTMS, OH1) [13, 14].

## 2. *p*-spectrum method

The proposed TDS-based *p*-spectrum method uses an external free standing module with a fiber-fed emitter and detector (Fig. 1a). This module is connected to the core unit of the Spectra 3000 from Teraview Company by means of optical fibers. The THz beam thanks to a set of the off-axis parabolic and flat mirrors is focused on the sample and after specular reflection is collected and focused on the detector. The investigations were carried out in the chamber filled with dry air (humidity less than 2%) and the distance between the sample and the mirrors was 30 cm. The incident angle of the beam illuminating the sample was 7 degrees. For these investigations, we manufactured the pellets having the diameter of 30 mm and various thicknesses by means of a

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hydraulic press, which ensured good flatness and smoothness of their surfaces. The fine powders of materials were mixed with a few percent of the phlegmatizing agent to mechanically stabilize the pellets.

Figure 1b presents the reference pulse with the FWHM equal to 0.4 ps reflected from the gold reference mirror. Figure 1c shows the fast Fourier transform (FFT) power spectra of the reference pulse and the noise level measured without the reference mirror. The dynamic range of the system is about 70 dB at 0.4 THz.
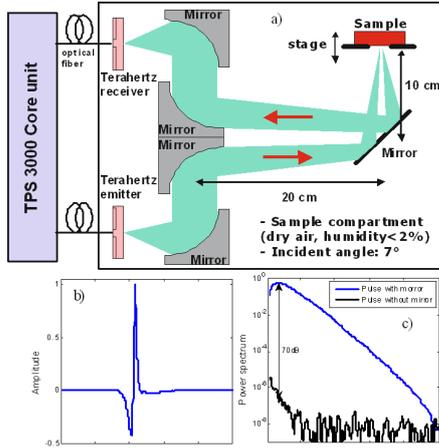


Fig. 1. Reflection measurement: simplified layout of the unit (a), the reference pulse (b), and power spectrum of the pulse with and without the reference mirror (c).

The proposed $p$-spectrum method for identification of the materials is based on the fact that the TDS signal reflected from a sample consists of a main peak and some "waves" after it, which carry the spectral information about the sample [11]. The FFT analysis of this part of the signal reveals some characteristic spectral features of the sample. Figure 2a and b shows the signal reflected from the smooth RDX sample (pellet). The red line represents only the part of the THz pulse (marked with the black line) which is analysed by FFT. The normalized power spectrum of this part of the pulse (called the $p$-spectrum) is shown in Fig. 2c. For comparison, we also present the absorbance of the RDX, which was measured in a transmission TDS setup and has a maximum at 0.84 THz [8]. The agreement of the frequencies of the peaks is very good.

It was also proved, both theoretically and experimentally, that we can analyze materials with spectral features in the range up to about 1.8 THz [11] using the above mentioned setup with the 0.4 ps FWHM pulses. Figure 3 presents the absorbance curves and the $p$-spectra of para--aminobenzoic acid (PABA) and sugar. The method is limited to about 1.8 THz because its sensitivity is associated with the spectrum of the incident pulse (see Fig. 1c): the higher the frequency the lower the signal, that explains the strong noise in the case of sugar (Fig. 3b). For the same reason, the $p$-spectrum peaks for PABA at
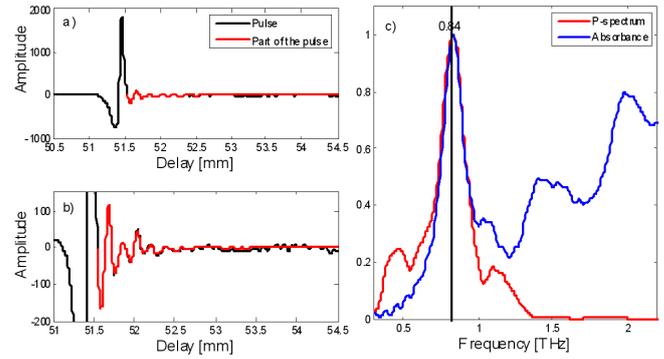


Fig. 2. The THz pulse reflected from the RDX sample (a), zoom-in of the Fig. 2a (b), and the $p$-spectrum (c).
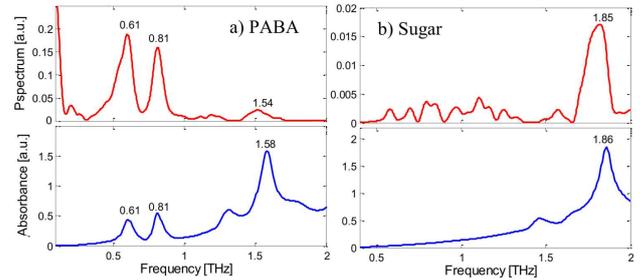


Fig. 3. The $p$-spectrum and the absorbance of: PABA (a) and sugar (b).

lower frequencies show larger amplitudes in comparison with those of higher frequencies.

### 3. Simulations and results

In order to assess parameters of the TDS pulse to investigate PETN and HMX, the following analysis was carried out. Let us assume a flat and smooth sample with the complex refractive index $N(\omega)$, which is illuminated at normal incidence with the electromagnetic pulse $E_0(t)$ presented in Fig. 1b. One can obtain the formula for the reflected pulse as

$$E_r(t) = F^{-1}\left(E_r(\omega)r(\omega)\right), \tag{1}$$

where $F^{-1}$ is the inverse numerical Fourier transform and $r(\omega)$:

$$r(\omega) = \frac{N(\omega) - 1}{N(\omega) + 1} \tag{2}$$

is the complex amplitude reflection coefficient.

For the purpose of simulations, we assumed pulses with FWHM equal to 0.4, 0.2 and 0.1 ps (Fig. 4). Their power spectra are presented in Fig. 5. Obviously, the shorter the pulse is, the broader is its spectrum. The pulse with FWHM equal to 0.1 ps has a broad and nearly flat spectrum in the range up to 2.5 THz.

Using the formula (1) and (2) we determined the reflected pulses and afterwards calculated the $p$-spectra
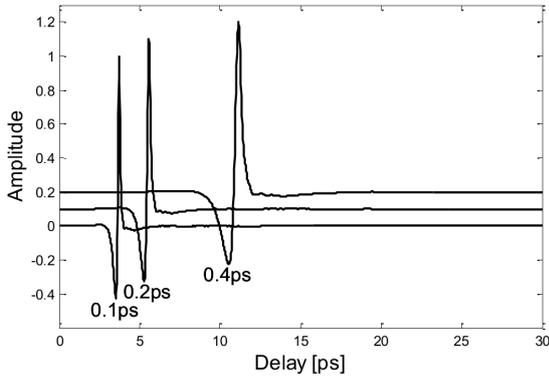
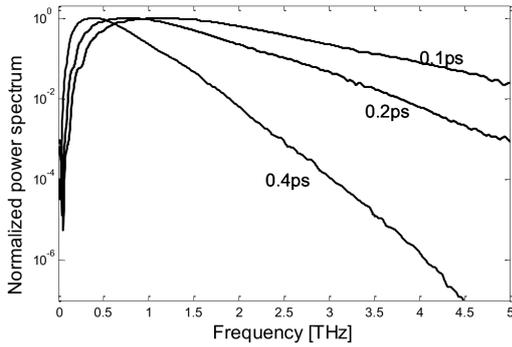Fig. 4.   The pulses used for simulations.



Fig. 5.   Normalized  power  spectra  of  the  pulses
from Fig. 4.



Fig. 7.   As in Fig. 6, but for PETN.



Fig. 8.   As in Fig. 6, but for HMX.

characteristics  by  means  of  the  concept  presented  in
Sect. 2.    For  the  calculations  we  used  four  materials:
sugar, PETN, HMX, and RDX.

In case of sugar (Fig. 6), one can notice that for the
incident pulse with FWHM = 0.4 ps the simulation re-
sults are comparable to the experimental ones presented
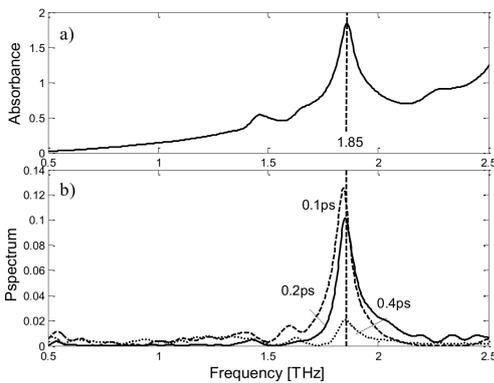in Fig. 3b.   The amplitude of the peak at 1.85 THz

reaches 0.02 in both cases.   For shorter incident pulses,
the $p$-spectrum peaks are higher and increase to about
0.1–0.12,  which  makes  the  identification  process  more
reliable.

It can be noticed in Fig. 7 and 8 that the incident pulses
with lower FWHM (and broader spectrum) improve vis-
ibility of the peaks in case of PETN and HMX. In case
of FWHM = 0.4 ps, the peaks at 2.02 THz and 2.18 THz
(PETN) and at 1.81 THz (HMX) are hard to notice, be-



Fig. 6.    Sugar: absorbance (a) and $p$-spectra calculated
for the incident pulses with FWHM = 0.1, 0.2, and
0.4 ps (b).



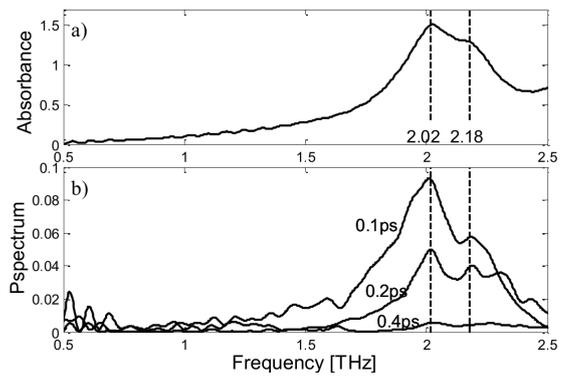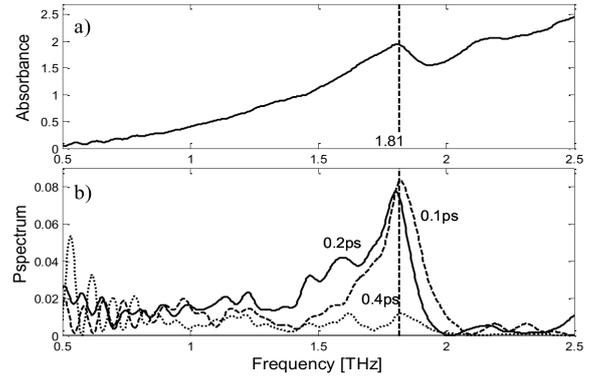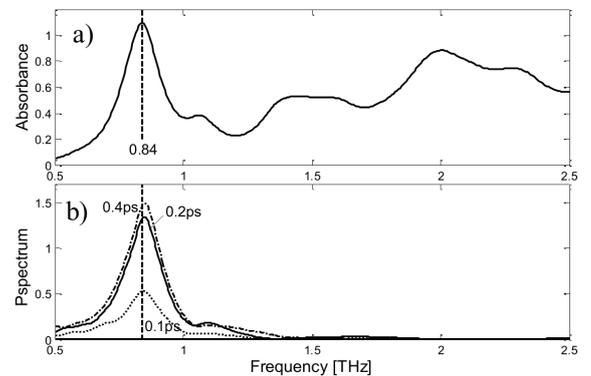Fig. 9.    As in Fig. 6, but for RDX.

cause their small amplitudes ($< 0.01$) are additionally suppressed by noise. In contrast, for lower FWHM values, the peaks are clearly seen with the amplitudes up to about 0.1.

Situation is different for RDX — the shorter the pulse duration, the smaller the amplitude of the peak at 0.84 THz in the *p*-spectrum characteristic (Fig. 9b). The maxima of the power spectrum of the pulses with smaller FWHM are shifted to the higher frequencies (Fig. 5), which causes visible decrease in the power for lower frequencies (below 1 THz).

## 4. Discussion and summary

In conclusion, we analyzed the limitations associated with the application of the *p*-spectrum method used to the extraction of the characteristic features of different materials. The described method is taking advantage of the available TDS arrangement with the pulse duration FWHM equal to 0.4 ps and is based on the analysis of the TDS pulse reflected from the sample. The spectrum curves of the available pulses decrease with frequency which limits the method to the frequencies up to about 1.8 THz. Therefore, RDX with peak at 0.84 THz can be easily investigated, while other important explosive materials such as PETN and HMX, with peaks at higher frequencies, are hard to analyze.

In this paper we theoretically proved that using the setup with a carefully designed bandwidth can significantly improve analysis of the explosives such as PETN and HMX. It can be concluded that pulse with FWHM around 0.15–0.20 ps is optimal for the *p*-spectrum method, taking into account the shape of the pulse assumed in the simulations, which is based on the pulses available in the pulse terahertz technology. In this case, the difference between the PETN and HMX peaks in the *p*-spectrum is sufficient for their reliable identification, while the decrease in case of the RDX peak is still not significant and does not obstruct its identification.

The TDS setups with pulses fulfilling the above mentioned requirements are currently available on the market and are based on the laser-induced gas plasma technique [12] or the TDS setups with organic crystals such as DAST, DSTMS, and OH1 [13, 14].

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