2D terahertz signatures for substance identification

By studying the time evolution of substances’ responses to terahertz radiation, materials of interest can be differentiated in a way not permitted by frequency domain analysis alone.

One of the most promising potential technologies for the detection and identification of explosives, drugs, and other dangerous substances is based on terahertz (THz) radiation.\textsuperscript{1–5} Terahertz time-domain spectroscopy (TDS) technology is based on analysis of absorption or reflection spectra in the terahertz range. Substances are detected and identified by comparing the spectrum of a pulse transmitted through the substance with a database of spectra.

However, we believe that this approach has at least three essential disadvantages. The first is related to the identification of simulants, substances with similar Fourier spectra at terahertz frequencies. THz-TDS does not allow, for example, identification of a substance hidden under a simulant cover or mixed with simulant material. The second is the lack of analysis of spectral lines that are absent in the initial pulse. Information about these spectral lines can be very important for finding explosives mixed with simulants. The third is the need to use a reference signal.

An alternative method of reliable identification uses estimates of terahertz pulse interaction with a medium over time. For this purpose, we proposed a few algorithms for dynamic analysis of the medium’s response spectrum under the action of a pulse with a few cycles, that is, the spectral dynamics analysis (SDA) method.\textsuperscript{6–13} This technique allows us to obtain the unique 2D signature of a substance at terahertz and gigahertz frequencies. The algorithms allow us to reconstruct the pulse shape on the basis of single value decomposition (SVD), for example, and to obtain the dynamics of many spectral lines on the time-frequency plane—the spectrogram—by one set of integral measurements. For long time intervals (100ps and more), the SDA method provides an opportunity to define the relaxation time for excited energy levels of molecules. This information can provide a new way to identify substances because the relaxation time differs for molecules of different substances. In comparison with autocorrelation or correlation functions and their spectra, the SDA method has better resolvability and provides much more accurate information about substances.

We used SDA to analyze experimental data for explosives, for mixtures of explosive with a neutral medium, and for explosives under an opaque substance, as well as for a mixture of a neutral substance with a small amount of simulant. Our

![Figure 1. Fourier spectra of terahertz signals transmitted through explosives (RDX and HMX) and opaque simulant covers: (a) RDX under a cotton cover (RDX_Cot_Air) and pure cotton (Cot_Air) and (b) HMX under a plastic cover (HMX_Plastic) and plastic alone.](image)
investigations showed that the spectrograms and dynamics of spectral lines in reflected and reference signals have fewer individual features (signatures) than in the case of identification using a signal transmitted through the substance. Nevertheless, we could determine the distinctions characterizing the presence of an additional substance in the sample and compare the transmitted and reflected signals. Therefore, the SDA method can be very effective for defense and security applications and also for quality control in the pharmaceutical industry. The following examples demonstrate its potential for substance detection and identification.

First, we examine explosives hidden under an opaque simulant cover. Pellets of RDX and HMX were covered with 1 mm-thick cotton or plastic. The Fourier spectra of terahertz signals transmitted through the pellets are shown in Figure 1.

Figure 2. Spectrograms for the signals of (a) RDX covered with cotton, (b) cotton, (c) HMX covered with plastic, and (d) plastic at terahertz frequencies.

Figure 3. Fourier spectra of (a) 5% L-tartaric acid and 5% sucrose within a polytetrafluoroethylene (PTFE) pellet (LTA5+Sucrose5) and (b) PTFE signals.

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A few differences appear only at $\nu > 1$THz. Specifically, we see two local minima at $\nu = 1.1$ and 1.8THz in Figure 3(a) that do not appear in Figure 3(b). Note that if we apply the autocorrelation function to calculate the spectra, these differences disappear.

In Figure 4, spectrograms for the LTA5+Sucrose5 and PTFE signals are shown for the frequency interval $0.8 < \nu < 3.6$THz. In Figure 4(a), two dark bands appear, one at the characteristic absorption frequency of L-tartaric acid ($\nu = 1.1$THz) and the other at that of sucrose ($\nu = 1.8$THz). Moreover, other absorption bands at $\nu = 2.64$ and 3.0THz for L-tartaric acid and at $\nu = 2.56$ and 3.4THz for sucrose are also apparent. In Figure 4(c) and (d), the spectral line dynamics at $\nu = 1.1$ and 1.8THz are depicted for the LTA5+Sucrose5 and PTFE signals. In Figure 4(c), the behavior of the spectral lines confirms that absorption occurs in the LTA5+Sucrose5 medium, whereas in Figure 4(d) the behavior is typical of transparency.

Next, we demonstrate the identification of L-tartaric acid by a reflected terahertz pulse. The signal reflected from a PTFE pellet containing a 10% concentration of L-tartaric acid (LTA_Refl) was

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measured over long time interval of about 320ps. Figure 5 shows the spectrograms of LTA_Refl and a reference signal over a long time interval of $500 \leq t \leq 820$ps. A high-intensity subpulse appears in both spectrograms after the main pulse, and two less intense subpulses are visible before the main pulse. The spectrograms differ during the main pulse: a dark absorption band occurs at $v = 1.2$THz in Figure 5(a) but not in Figure 5(b). Moreover, they also differ during the bright subpulse, which is more intense in Figure 5(a) than in Figure 5(b). The evolution of spectral lines at low frequencies ($v = 0.23$ and 0.41THz) also appears in Figure 5. We can see very intense re-radiation of the terahertz energy before and after the main pulse action for the LTA_Refl signal in Figure 5(c), whereas in the reference signal in Figure 5(d), the re-radiation is several times less intense.

The SDA method is a very effective tool for detecting and identifying substances by using a terahertz pulse reflected from or transmitted through them. It can be very effective for security applications and for remote quality control. To increase the accuracy of identification, we plan to make further simultaneous measurements of a signal over a wide angular range. This would also provide information about a substance’s absorption characteristics.

**Figure 5.** Spectrograms of the (a) LTA_Refl and (b) reference signals over a long time interval ($500 \leq t \leq 820$ps) and (c, d) the dynamics of their spectral lines at $v = 0.23, 0.41$THz.

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**References**