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A phase feature extraction technique for terahertz reflection spectroscopy

Hua Zhong,¹ Cunlin Zhang,¹ Liangliang Zhang,^{1,2,a)} Yuejin Zhao,² and Xi-Cheng Zhang³

¹Beijing Key Lab for Terahertz Spectroscopy and Imaging, Key Laboratory of Terahertz Optoelectronics, Ministry of Education, Capital Normal University, No. 105 XiSanHuan BeiLu, Beijing 100037, People's Republic of China

²Department of Optical Engineering, Beijing Institute of Technology, Zhongguancun Nandajie 5, Beijing 100081, People's Republic of China

³Center for THz Research, Rensselaer Polytechnic Institute, Troy, New York 12180, USA

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We present a feature extraction technique for identification of explosive and biological materials using terahertz reflection time-domain spectroscopy (RTDS). The absorption signatures of the materials are extracted directly from the second-order derivative of the phase of the sample beam with respect to frequency. This technique provides a straightforward and fast solution to solve the phase-retrieval problem in RTDS and will benefit the future development of a standoff, large-size focal-plane terahertz sensing and imaging system. © 2008 American Institute of Physics.

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The terahertz band offers a plethora of fingerprints for many chemical and biological materials. Within the past few years, efforts have been focused on exploiting the broadband nature of the terahertz time-domain spectroscopy (TDS) system for materials identification and characterization.^{1–5} terahertz-RTDS has been envisioned as a more practical measure by allowing three-dimensional reconstruction of layered structures and being the only way to inspect terahertz-opaque targets.^{6,7}

Generally, a terahertz-RTDS measurement requires a sample beam and a reference beam.⁸ In particular, the retrieval of phase shift caused by absorption has been a bottleneck, because the “misplacement phase error”—ranging difference between the reference beam and sample beam—is hard to correct.⁹ Various methods have been proposed to solve this problem.^{10–13} Most of the methods require human intervention or a large amount of computation. More importantly, they are not suited to a setup where atmospheric attenuation has to be included.¹⁴

In this work, we propose a feature extraction technique for RTDS, which is able to remove the phase error without any human intervention by taking advantage of the almost-linear phase spectrum of terahertz pulses.¹⁵ In an ideal case ignoring atmospheric absorption, this method is reference free. We are aware that the reference-free measurement of complex refractive index can also be done by taking the amplitude of both polarizations.¹²

The spectral phase, derived from a typical time-domain terahertz waveform by Fourier transform, is essentially linear.¹⁵ As the terahertz wave is reflected upon the target surface after traveling for a pathlength of L in the air, its phase φ_s is governed by

$$\varphi_s(\omega) = \varphi_0 + \omega n_{\text{air}} L/c, \quad (1)$$

where φ_0 is the phase change caused by the material absorption, ω is the angular frequency, n_{air} is the refractive index of the air, and c is the speed of light. n_{air} is generally regarded as a constant at a low humidity level.¹⁶ It has been demonstrated elsewhere that for a weakly polarized organic com-

pound (such as explosives and related compounds, biochemicals, etc.), the extinction coefficient κ can be determined directly from φ_0 by the following approximation:^{13,17}

$$\varphi_0 = \tan^{-1} \left(\frac{2\kappa}{n_{\infty}^2 + \kappa^2 - 1} \right) \sim \tan^{-1} \left(\frac{2\kappa}{n_{\infty}^2 - 1} \right), \quad (2)$$

where n_{∞} is a constant. From Eq. (1), under the assumption of a weakly polarized organic compound, the first-order derivative of the sample beam phase is determined by

$$\frac{d\varphi_0}{d\omega} = \frac{2}{(n_{\infty}^2 - 1)[1 + 4\kappa^2/(n_{\infty}^2 - 1)^2]} \frac{d\kappa}{d\omega} \sim \frac{2}{(n_{\infty}^2 - 1)} \frac{d\kappa}{d\omega}. \quad (3)$$

As a result

$$\frac{d^2\varphi_s}{d\omega^2} = \frac{d^2\varphi_0}{d\omega^2} \sim \frac{2}{(n_{\infty}^2 - 1)} \frac{d^2\kappa}{d\omega^2}. \quad (4)$$

Using a numerical method similar to the one used in Ref. 13, it can be shown that for a weakly polarized organic compound, $d^2\kappa/d\omega^2$ bears a similar shape with κ (but is negative). This close relationship between κ and its double derivative is rooted in Kramers–Kronig relation.¹⁷ That means when n_{air} can be approximated as a constant, $d^2\varphi_s/d\omega^2$ alone contains the absorption features of the chemical. However, when the water vapor absorption cannot be neglected, Eq. (4) becomes

$$\begin{aligned} \frac{d^2\varphi_s}{d\omega^2} &\sim \frac{2}{(n_{\infty}^2 - 1)} \frac{d^2\kappa}{d\omega^2} + \frac{L}{c} \left(2 \frac{dn_{\text{air}}}{d\omega} + \frac{d^2n_{\text{air}}}{d\omega^2} \right) \\ &\sim \frac{2}{(n_{\infty}^2 - 1)} \frac{d^2\kappa}{d\omega^2} + \frac{2L}{c} \frac{dn_{\text{air}}}{d\omega}. \end{aligned} \quad (5)$$

As a result, a reference beam with phase φ_r has to be applied to remove the second term so that

$$\frac{d^2(\varphi_r - \varphi_s)}{d\omega^2} \sim \frac{2}{(n_{\infty}^2 - 1)} \frac{d^2\kappa}{d\omega^2} + \frac{2\delta L}{c} \frac{dn_{\text{air}}}{d\omega}, \quad (6)$$

where δL is the ranging difference between the reference surface and sample surface. It is noteworthy that the distur-

^{a)}Electronic mail: zhlliang@126.com.

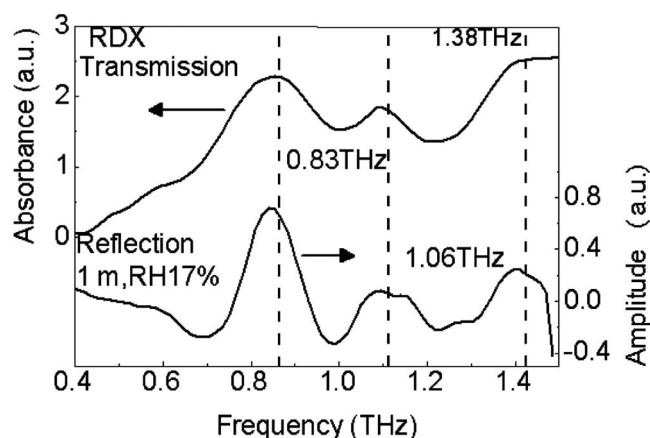


FIG. 1. Measurements of RDX. Top: absorbance taken in nitrogen-purged transmission setup (contrast). Bottom: $d^2(\varphi_s - \varphi_r)/d\omega^2$ taken under a humidity level of 17%, at 1 m away (the curve is flipped to be positive). Dotted lines indicate the confirmed absorption lines around 0.83, 1.06, and 1.38 THz.

tions caused by this term only center around water absorption lines. As long as the absorption peak of the target lies between two water lines, this term does not affect the shape of the phase feature. In our system, we will show that at a standoff sensing distance of 5 m (10 m total traveling distance), under a high humidity level of 37%, a δL less than 20 mm does not introduce any significant error to the final results. This provides the feasibility of using reflection from the vicinity of the target (human skin, vehicle surface, etc.) as reference in future standoff sensing modalities.

The experimental setup has been described in our previous work.¹⁸ In this work, the single trip of the terahertz pulse varies from 1 to 5 m. The samples being measured are hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), 2,4-dinitrotoluene (2,4-DNT), and theophylline, which are all compressed pellets with a thickness of ~ 1.5 mm and a diameter of 13 mm. All the sample powders were ground to a grain size smaller than $50 \mu\text{m}$ to avoid scattering. The reference reflector is a metal mirror with a thickness of ~ 10 mm, introducing a maximum $\delta L \sim 2 \times 10 = 20$ mm. The time-domain terahertz waveforms were taken within a uniform window of 20 ps to avoid the backside reflection.

Figure 1 shows the measured results of RDX plotted in linear scale with arbitrary unit. The top one provides the contrast, which is the absorbance measured by standard

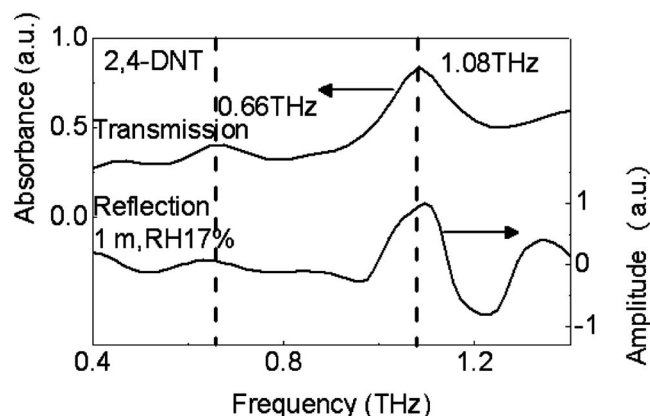


FIG. 2. Measurements of 2,4-DNT, at the same conditions as Fig. 1. Dotted lines indicate the confirmed absorption lines around 0.66 and 1.08 THz.

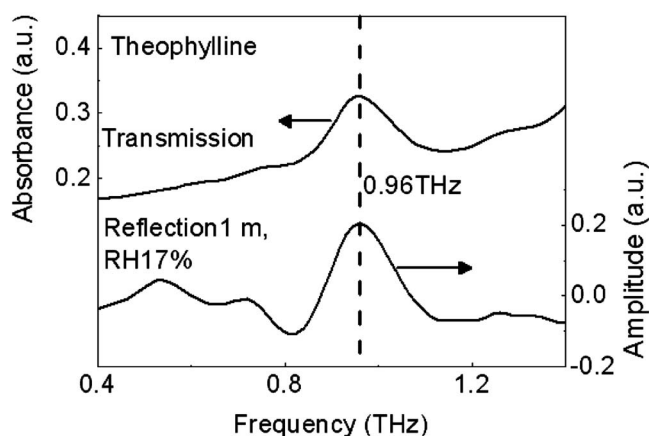


FIG. 3. Measurements of theophylline, at the same conditions as Fig. 1. Dotted line indicates the confirmed absorption line around 0.96 THz.

transmission setup in a separate nitrogen-purged cell. All the marked absorption lines on the transmission data have been confirmed by other groups.¹⁻⁴ The curve on the bottom is the spectrum of $d^2(\varphi_s - \varphi_r)/d\omega^2$ taken under RH (relative humidity) of 17%, measured when the target is ~ 1 m away from the generation and detection unit (the curve is flipped to be positive). A reference beam reflected from a metal mirror is used to eliminate the phase shift caused by water vapor absorption. The results show that the marked absorption peaks of RDX around 0.83, 1.04, and 1.38 THz on the transmission data are all seen on the reflection one using our method. Figure 2 gives the measured results of 2,4-DNT at the same conditions. The absorption peaks around 0.66 and 1.08 THz are clearly identified. Figure 3 is the results of theophylline at the same conditions. The peak at 0.96 THz is found. The tiny ripples before the 0.96 THz peak on the reflection curve are sitting around water lines (0.56 and 0.75 THz). They are likely caused by humidity vibration that occurred during the measurement. It is noted that the absolute values of absorbance on Figs. 1–3 are not used but can be found in Ref. 16.

Figure 4 compares the results of RDX under different humidity levels and distances (the curves are flipped to be positive). From top to bottom, the curves are $d^2(\varphi_s - \varphi_r)/d\omega^2$

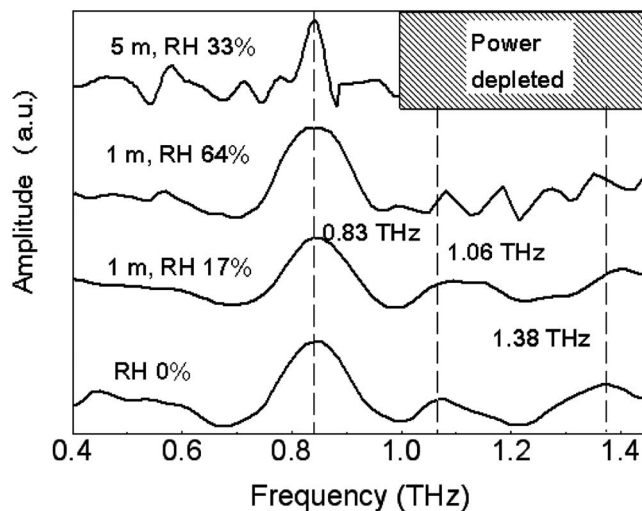


FIG. 4. Results of RDX measured under different humidity levels and distances. From top to bottom: $d^2(\varphi_s - \varphi_r)/d\omega^2$ at 5 m, RH 33%; $d^2(\varphi_s - \varphi_r)/d\omega^2$ at 1 m, RH 64%; $d^2(\varphi_s - \varphi_r)/d\omega^2$ at 1 m, RH 17%; $d^2\varphi_s/d\omega^2$ in a separate nitrogen-purged cell, RH 0% (the curves are flipped).

$-\varphi_r)/d\omega^2$ measured at 5 m away from the unit under RH 37% (water absorption has depleted the terahertz power beyond 1 THz so it is covered by a shaded area); $d^2(\varphi_s - \varphi_r)/d\omega^2$ measured at 1 m away, under a high RH of 64%; $d^2(\varphi_s - \varphi_r)/d\omega^2$ measured at the same distance, under RH 17%; and $d^2\varphi_s/d\omega^2$ measured in a separate nitrogen purged cell. All three peaks are clearly shown on the reference-free curve $d^2\varphi_s/d\omega^2$. As the humidity level goes up, the baseline becomes noisier, the peaks around 1.04 and 1.38 THz are less prominent. Eventually, they die off at RH 64%. This feature degrading is explained by a higher vibration of the water vapor concentration as the humidity level increases. On the other hand, at 5 m, the peak at 0.83 THz is still seen but has become narrower with more noises on the background due to poorer signal-to-noise ratio (SNR) at longer distance. Taking double derivative on phase, the proposed method does place stricter requirement on SNR than conventional method.¹⁸ However, in an open field, the system could be more tolerant by using faster delay line and removing all the multiple reflectors.

Our results show that in most cases it is still necessary to apply a reference beam to remove the noise from the water vapor absorption and the system. Nevertheless, by using this method, in all measurements the misplacement phase error δL does not affect the extraction of the absorption feature at all. It is noteworthy that current setup is yet to know if terahertz RTDS is able to identify samples with more loosely confined surface morphology, such as powder or chunk, but other work suggests the possibility.¹³

In conclusion, we present a phase feature extraction technique for weakly polarized organic compounds in stand-off terahertz RTDS by taking the second-order derivative of the phase of the signal beam with respect to frequency. In nitrogen purged environment, this method does not require any reference. In real scenarios, a reference beam is applied only to remove the influence of atmospheric attenuation. This method offers a straightforward and speedy way to retrieve the reflective absorption features without the presence

of the amplitude of the terahertz pulse or the settlement of a reference surface.

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