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# Terahertz Time-Domain Spectroscopy method for optical parameter extraction of plastic materials

ZHANG Dandan, REN Jiaojiao, LI Lijuan, CAO Guohua  
(Changchun University of Science and Technology, Changchun Jilin 130022, China)

**Abstract:** A method for extracting optical parameters of plastics materials based on terahertz time domain spectroscopy is presented. The transmission-type Terahertz Time-Domain Spectroscopy (THz TDS) system is adopted to detect the refractive index and extinction coefficient on different plastic materials. Then the corresponding spectral information is obtained by Fourier transform of the terahertz time domain waveform of the sampling points, including the corresponding amplitude and phase information of the waveform. The optical parameter extraction model is built. By using the simplex optimization method, the curves of the refractive index and extinction coefficient for the plastic material are obtained. The experimental samples are made of different plastic parallel plate materials. The experimental results show that the optimization of optical parameters can improve their extraction accuracy, and the error of refractive index is  $\pm 0.005$ . Extraction technology with the simplex optimization method of optical parameter based on THz TDS can help to extract the optical parameters of engineering plastics. It is of great significance for the research of terahertz nondestructive testing.

**Keywords:** Fourier transform; Terahertz Time-Domain Spectroscopy; optical parameters; refractive index; extinction coefficient

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## 1 Introduction

Now, kinds of spectroscopic techniques have been widely used in the analysis of matter. Terahertz (THz) wave usually refers to the electromagnetic radiation of frequency between 0.1 THz and 10 THz (wavelength of 30  $\mu\text{m}$ ~3 mm), which is between the microwave and infrared<sup>[1]</sup> in the electromagnetic spectrum. It has a good permeability to many dielectric materials and non-polar materials, with pico-second time resolution, and it will not damage the tested materials for its photon energy radiation is low. Therefore, THz technology has been rapidly developed and applied in the field of nondestructive testing<sup>[2-3]</sup>. It can be utilized to detect the physical and chemical characteristics of a variety of materials (such as insulator, semiconductor and liquid), and it can also identify the material properties and structure information by analyzing the spectral imaging. THz TDS has become a new method of spectral analysis, which is a hot spot in the field of material analysis.

THz TDS is a new technique for the measurement of the spectral components in the far infrared band based on the ultrafast laser. The composition and structure of the material can be reflected by the characteristic absorption analysis by THz radiation. The optical parameters of the non-polar materials such as engineering plastics obtained by the transmission-type THz TDS, on a macroscopic scale, characterize the optical properties of materials physically, which indirectly reflects the microstructure and properties of these materials<sup>[3]</sup>.

This paper adopts different plastic material plates as the samples, utilizes the TDS detection system to build the transmission-type measurement platform, and perform the detection of engineering plastics plate materials. The refractive index and extinction coefficient of the material are also analyzed through THz TDS. Then, the optical parameters extracted for the plastic material are optimized by using the simplex method, which improves the extraction precision. Exaction technology of optical parameter based on THz TDS, provides a basic guarantee for the application of terahertz nondestructive

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testing of engineering plastics, and also provides data support for the establishment of the optical parameters database of engineering plastics in terahertz band.

## 2 Experimental Setup

Extraction technology of optical parameter based on THz TDS is a coherent detection technology<sup>[4]</sup>. A schematic of a transmission-type THz TDS measurement system is shown in Fig.1. High speed femtosecond laser pulses excite terahertz source to generate terahertz pulses, and the other part plays a role of detection. The probe light passes through the time delay control system, and goes through the terahertz detection element together with the terahertz pulse. Time delay system is adopted to make the probe light execute a real-time sampling of the intensity information of terahertz pulse. It can change the optical path difference between the probe light and terahertz pulse, so as to obtain terahertz time-domain waveform<sup>[5]</sup>. The terahertz wave is emitted by the transmitting device(transmitter), then passes through the tested plastic sample, and is received by the receiving device(receiver)<sup>[6]</sup>.

The plastic sample is placed in middle position between the emission devices and the receiving device, the planar dimensions of plastic samples are 50 mm×50 mm. Samples include 5.23 mm High Density Polyethylene(HDPE), 14.9 mm Poly Propylene(PP) polypropylene, 5.2 mm Poly Tetra Fluoro Ethylene(PTFE) Teflon, 15.28 mm Poly Ethylene(PE) polyethylene and 3.2 mm Poly Amide(PA) polyamide.

## 3 Optical Parameter Extraction Model

### 3.1 Optical Parameter Extraction Model of Transmission-type THz TDS

For the extraction of the optical parameters of engineering plastic material by using transmission-type THz TDS system, the basic principle of the extraction technology is using the femtosecond pulse to generate terahertz electric field. Then collecting the transmission spectrum information after the terahertz wave passing through materials, the amplitude and phase information can be obtained. Through the Fourier transform of the time-domain waveform, the spectral information of the tested materials can be directly obtained. The traditional parameter extraction formula is<sup>[7-8]</sup>:

$$\tilde{n}(\omega) = \frac{c\Delta\varphi(\omega)}{\omega d} + 1 \quad (1)$$

$$\kappa(\omega) = \frac{c}{\omega d} \ln \frac{4\tilde{n}(\omega)}{\sqrt{T_{\text{sample}}(\omega)}[\tilde{n}(\omega) + 1]^2} \quad (2)$$

Where,  $\tilde{n}(\omega)$  is the real refractive index of sample;  $\kappa(\omega)$  is the extinction coefficient of sample;  $\Delta\varphi(\omega)$  is the phase change after terahertz wave passing through the sample;  $T_{\text{sample}}(\omega)$  is the power of terahertz wave after passing through the sample;  $\omega$  is the angular frequency of terahertz wave;  $d$  is the thickness of the tested sample;  $c$  is the propagation velocity of terahertz wave in vacuum.

In the actual measurement process, when terahertz wave spreads in the sample, Fabri Perot effect will be generated in the interface between air and sample. At the same time, because the traditional formula is under the condition of thicker samples, it has ignored the multiple reflections phenomenon. So if the refractive index and extinction coefficient of the sample are calculated by using the traditional parameter extraction formula, a large error will be caused. Therefore, it is necessary to optimize the parameter extraction model. Fig.2 shows the transmission diagram of vertically incident terahertz wave in the sample.

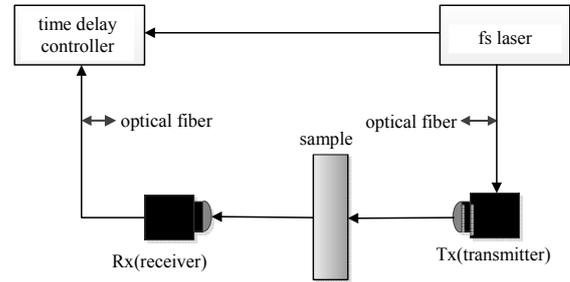


Fig.1 Transmission-type THz TDS measurement system

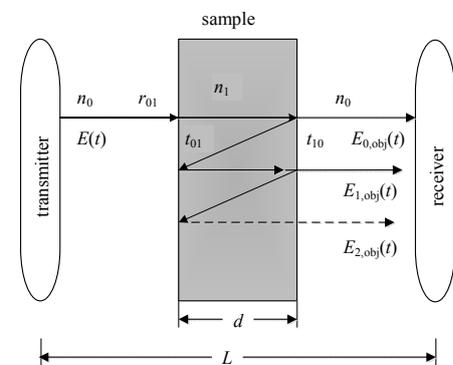


Fig.2 Transmission-type THz TDS propagation model

Therefore, it is necessary to optimize the parameter extraction model. Fig.2 shows the transmission diagram of vertically incident terahertz wave in the sample.

As shown in the Fig.2, the terahertz signal is emitted from the transmitter. At the interface between the sample and air, multiple reflections occur when terahertz signal passes through the sample. Therefore, the receiver receives the superposed terahertz signals include the signal transmitted directly through the sample and the multiple reflected signals. The received terahertz  $E_{obj}(t)$  signal is composed of  $E_{0,obj}(t), E_{1,obj}(t), E_{2,obj}(t)$ . When the original terahertz signal  $E(t)$  passes through the plastic sample, the signal  $E_{obj}(t)$  will be obtained. Here,  $E_{ref}(t)$  is taken as the reference signal to denote the terahertz signal without passing through the sample.

The terahertz signal having passed through the plastic sample contains multiple reflected signals.

In this paper, only three reflected terahertz signals are listed. The terahertz signal having passed through the plastic sample can be expressed as:

$$E_{obj}(\omega) = E_{0,obj}(\omega) + E_{1,obj}(\omega) + E_{2,obj}(\omega) + \dots = E(\omega)p_{ref}(\omega)t_{01}p_{obj}(\omega)t_{10} + E(\omega)p_{ref}(\omega)t_{01}p_{obj}(\omega)t_{10}r_{10}^2p_{obj}^2(\omega) + E(\omega)p_{ref}(\omega)t_{01}p_{obj}(\omega)t_{10}r_{10}^4p_{obj}^4(\omega) + \dots \tag{3}$$

Where,  $p_{ref}(\omega)$  is the phase change function without the sample;  $p_{obj}(\omega)$  is the phase change function with the sample;  $t_{01}$  and  $r_{10}$  are the transmission coefficient in the air and the reflection coefficient in the sample interface respectively.

Where,  $E_{ref}(\omega) = E(\omega)p_{ref}(\omega)$ , so the transfer function of transmission-type measurement theory can be obtained. The transmission-type transfer function is obtained through the convolution between the sample signal and the reference signal and filtering, it can be expressed as the theoretical ratio between the terahertz spectrum of the sample signal and reference signal<sup>[9]</sup>.

$$H(\omega) = \frac{E_{obj}(\omega)}{E_{ref}(\omega)} = t_{01}p_{obj}(\omega)t_{10} \left\{ 1 + \sum_{k=1}^2 [r_{10}^2 p_{obj}^2(\omega)]^k \right\} = \frac{4\tilde{n}(\omega)}{(1 + \tilde{n}(\omega))^2} \exp \frac{-j(\tilde{n}(\omega) - 1)\omega d}{c} \left\{ 1 + \sum_{k=1}^2 [r_{10}^2 p_{obj}^2(\omega)]^k \right\} \tag{4}$$

Where,  $\tilde{n}(\omega) = n(\omega) - j\kappa(\omega)$  is the negative refractive index.

To definite  $FP(\omega) = 1 + \sum_{k=1}^2 [r_{10}^2 p_{obj}^2(\omega)]^k$ , here,  $k$  is an integer, which denotes the echo level,  $k=0$  says the main echo. It is the function coefficient due to Fabri Perot effect.

### 3.2 Optical Parameter Optimization

In this paper, the simplex method is adopted to optimize the optical parameters, and the optimization steps are shown in Fig.3. Where, one degree error functions are the real refractive index  $\tilde{n}(\omega)$  and the extinction coefficient  $\kappa(\omega)$ . The error function is:

$$\delta(\omega) = \sum_{\omega} |mER(\omega)| + |pER(\omega)| \tag{5}$$

Where,  $|mER(\omega)|$  is the amplitude error of transfer function,  $|pER(\omega)|$  is the phase error of transfer function, containing the difference between the amplitude and the phase of the theoretical transfer function and the actual transfer function. The error function works as the fitness function of the simplex method. So the original refractive index is

$n_{initial} = \frac{\Delta t \cdot c}{d} + 1$ , the original extinction coefficient is  $\kappa_{initial} = 0$ , Where,  $d$  is the sample's thickness,  $\Delta t$  is the time delay of the sample signal  $E_{obj}(t)$  and reference signal  $E_{ref}(t)$ .

Nelder and Mead simplex optimization algorithm does not perform any derivation operation, and the algorithm is relatively simple. In this paper, it is applied to the optimization of the real and imaginary parts of refractive index. The basic idea is to replace the worst vertex in the error function through implementing reflection, extension, contraction and compression on the triangle which consists of three vertices in a two-dimensional space; and to throw the vertex responding to the worst, and then form a single new shape with the new vertex, gradually approaching the best responding point.

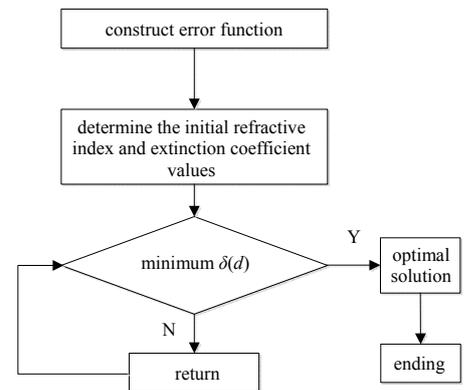


Fig.3 Simplex method optimization steps

#### 4 Material Parameter Extractions

The accuracy of the simplex algorithm about the refractive index and extinction coefficient is affected by the uncertainty of the measured signal. Because of the multiple reflections phenomenon inside the sample, if the time window of the signal acquisition is limited, the echo number in the time window is not an integer, the signal cannot completely reflect the signal characteristics. Then the uncertainty of measured signal makes the optical parameter calculation cannot be performed directly. In this paper, the simplex method is utilized to optimize and revise the optical parameters, which improves the accuracy and reliability of the results. The refractive index curves are shown in Fig.4, and the extinction coefficient curves are shown in Fig.5.

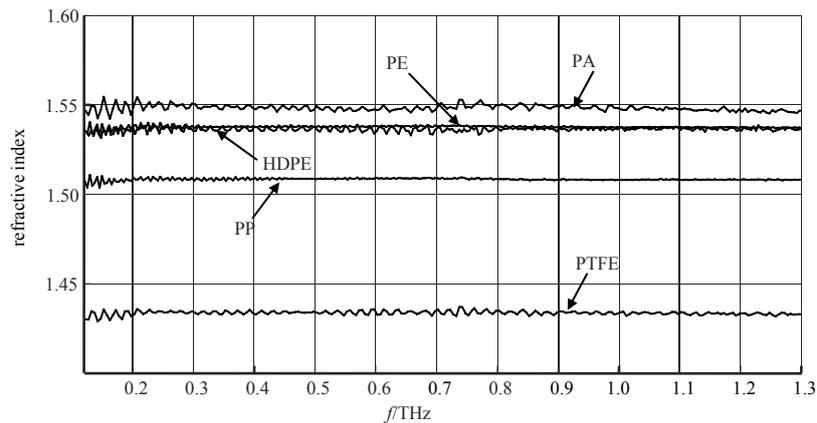


Fig.4 Refractive index curves of engineering materials

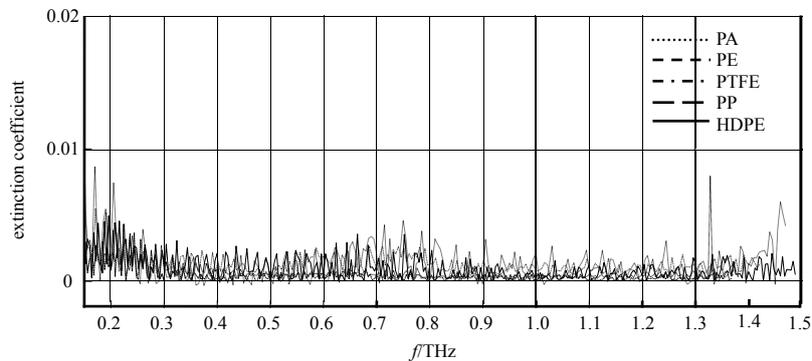


Fig.5 Extinction coefficient curves of engineering plastics

As shown in Fig.4 and Fig.5, the measured refractive indexes of the optimized HDPE, the optimized PP, the optimized PTFE, the optimized PE, and the optimized PA materials are about 1.535 in the 0.2–1.3 THz band, 1.508, 1.436, 1.538, 1.549, respectively. The error of refractive index is  $\pm 0.005$ , and the results are consistent with the previous references, which proves that the method is feasible and effective. The results of parameter extraction are shown in table1.

#### 5 Conclusion

Through the analysis, the transmission-type THz-TDS can be adopted in the extraction of optical parameters for engineering plastics and other non-polar materials. Using the simplex optimization algorithm can effectively improve

the accuracy of the refractive index and the extinction coefficient, and solves the problem that multiple reflections will cause large parameter error in the process of optical parameter extraction. If the extracted optical parameters are applied in the analysis of the terahertz time-domain and frequency-domain imaging, the material internal defects can be identified

Table1 Refractive index of engineering plastics

engineering plastic material	thickness/mm	refractive index
HDPE high density polyethylene	5.23	$1.535 \pm 0.005$
PP polypropylene	14.90	$1.508 \pm 0.005$
PTFE teflon	5.20	$1.436 \pm 0.005$
PE polyethylene	15.28	$1.538 \pm 0.005$
PA polyamide	3.20	$1.549 \pm 0.005$

more accurately, which has great significance on the study of nondestructive detection of THz TDS, and provides data support for terahertz optical parameter database being standardized.

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#### About the authors:



**ZHANG Dandan**(1990–), female, was born in Changchun, Jilin province. Doctor degree. The main research direction is terahertz nondestructive testing,email:zhangdandan\_rita@126.com.

**CAO Guohua**(1965–), male, was born in Jiamusi, Heilongjiang province. Doctor degree. The main research directions include mechanical and electronic engineering.

**REN Jiaojiao**(1988–), female, was born in LYUliang, Shanxi province. Doctor degree. Her main research direction is terahertz nondestructive testing.

**LI Lijuan**(1972–), female, was born in Nanyang, Henan province. Doctor degree, professor. Her main research directions are opto–electronic precision measurement, digital assembly and nondestructive testing.