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Practical method to estimate the standard deviation in absorption coefficients measured with THz time-domain spectroscopy

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ABSTRACT

A model of standard deviation in the intensity spectrum of electric field observed with the terahertz time-domain spectroscopy (THz-TDS) is proposed to estimate the random error in the transmittance and absorption coefficients from a single or a few measurements of a sample. The proposed standard deviation which is derived on the basis of the statistical standard deviation and noise floor of intensity spectrum of reference fits well to the standard deviation of transmittance as well as absorption coefficient computed statistically. This study contributes the simple and computationally efficient method to demonstrate the accuracy in optical constants like imaginary part of refractive index and absorption coefficients measured using the THz-TDS.

1. Introduction

Terahertz time-domain spectroscopy (THz-TDS) has been widely used to study the spectroscopic characteristics of the variety of the materials [1–3] like dielectrics [4], semiconductors [4,5], bio-molecules [6], liquids [7], pharmaceutical products [8] and so on in the spectral region spanning from 0.1 to 3 THz. Most spectroscopic measurements involve the recording of a time-domain pulse of THz electric field transmitted through a sample under investigation placed on the path of the terahertz radiation and a reference signal recorded in the absence of the sample. The time-domain waveforms are converted to the frequency-domain by the complex Fourier transform to obtain the intensity and phase spectra. These spectra are processed further to calculate the transmittance and phase differences which are used to derive the frequency dependent dielectric properties like complex refractive index, complex dielectric constant and absorption coefficient.

The measured spectra of sample and reference electric fields using THz-TDS and the dielectric properties (also called as optical constants) obtained using these electric fields are prone to have systematic and random errors and the precision is limited by them (e.g., see Ref. [9]). The systematic error is due to error in measure of sample-thickness measurements (including parallelism and roughness of the surfaces), sample misalignment, error in optical delay distance, etc. and these errors could be eliminated or reduced to some extent by making effort in sample preparation, spectrometer calibration and so on. However, the random errors which are caused mainly by laser power fluctuation, electronic noise in devices, optical and mechanical instability cannot be removed completely and it becomes necessary to quantify them with statistical analysis by taking number of observations.

Previously, a method to identify the dynamic range from one reference spectrum and the detectable limit of absorption coefficient from the sample spectrum has been reported [10], but this does not provide the information on the random error in measured data. The methodology to determine the standard deviation in intensity spectrum has been reported by taking large number of measurements [11]. As one scan of measurement in THz-TDS requires several to ten minutes, more than several hours are necessary to take enough number of sample and reference data for evaluating the statistical standard deviations in the measured optical parameters with an ordinary frequency resolution, which is usually difficult and not practical to execute always for many samples. One or a few pair of reference and sample data are usually expected to obtain the optical parameters of each sample by the THz-TDS, in which case the estimation of errors cannot be done by statistical methods. Therefore, in this study we provide the method to estimate the error in the transmittance and absorption coefficient even if a sample is measured only one time with THz-TDS by using the statistical standard deviations in the intensity spectra derived from many number of reference data.

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2. Measurements

We took a number of reference and sample time-domain waveforms with a THz-TDS system to examine the error characteristics in the measured data. The THz-TDS system used for the measurement is the Rayfact SpecTera [12] (Tochigi Nikon Corporation) consisting of a compact femto-second fiber laser (Femtolite, IMRA Inc.) with a pulse width of <100 fs and 20 mW average power and LT-GaAs photoconductive antennas as THz emitter and detector. Three ZnTe crystals with different thickness (0.767, 1.496 and 2.976 mm) supplied commercially by Nippon Mining and Metals Co. Ltd. [13] are used as samples and they have very low absorption coefficient in the frequency range of 0.2–3 THz [14]. The time-domain data of 1024 points is taken in one scan of time delay line with the frequency resolution of 0.024 THz (0.814 cm^{-1}), which needs about 10 min for each scan. The data is observed in the sequence like $R_0, S_0, S_1, R_1, R_2, S_2, \ldots, R_k, S_k, \ldots, S_{m-1}, S_m, R_m$, where R and S are the reference and sample data respectively, and k and m of subscripts are integers. The R_k and S_k with the same subscript means a pair of reference and sample data which are close to each other in time at which they are measured. Twelve, 16 and 16 data sets of reference and sample waveforms were recorded for the 0.767, 1.496 and 2.976 mm-thick ZnTe crystal respectively.

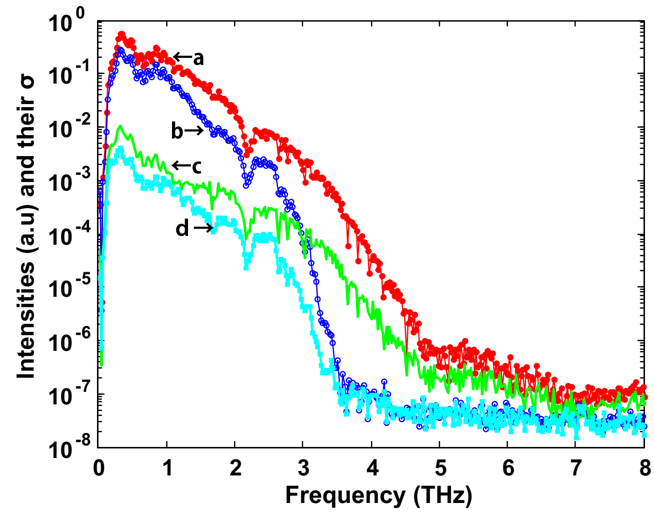

Fig. 1. Frequency-domain reference and sample signals and their standard deviations. Curves (a) and (b) show the averaged intensity spectra of the reference and sample and curves (c) and (d) are their respective standard deviations.

3. Derivation and modeling of standard deviation

The time-domain pulses of electric field suffered from the random error are characterized by the temporal shift of pulse position and pulse shape, which are approximately represented by a position in time and amplitude of the largest pulse in the waveform respectively. The variation in position and amplitude of the peak depend on time of an order of hour, which showed good correlation between reference and sample data. It is possible to correct the variation in position and amplitude of the largest peak pulse by performing a data processing prior to taking Fourier transform. We, therefore, adjusted the waveforms so that respective peak amplitude becomes equal to the averaged peak height. After conversion of the waveform data from time-domain to frequency-domain by the Fourier transform, this pre-processing have brought a good effect to improve the standard deviation in the intensity spectra. As a result, the standard deviation in the transmittance derived through the error-propagation from reference and sample spectra has become almost equal to the statistical standard deviation which is calculated from the transmittances obtained using each pair of reference and sample spectra. In other words, this means the data taken more closely in time has smaller variance.

The intensity spectra of reference and sample are derived by the procedure explained above for the ZnTe crystals with three different thicknesses. Fig. 1 displays the average of 12 data of 0.767 mm ZnTe sample and reference spectra along with their respective standard deviations calculated by statistical mathematics. Beyond the detectable upper frequency limit, the intensity spectrum approaches a flat noise level, which is called as the noise floor [10,15]. The intensity spectra of reference and sample have the noise floor above 7 and 4.5 THz respectively. The remarkable feature in Fig. 1 is that the standard deviations of reference and sample are much higher than the level of noise floor in the larger intensity region and they are correlated with the respective intensity; the intensity of the sample is smaller than that of the reference due to attenuation caused by the ZnTe crystal and hence the standard deviation of former is smaller than latter's. Spectra of intensity and standard deviation of the reference as well as sample show that the signal-to-noise ratio (SNR) is rapidly improved with an increase in the intensity from the noise floor to a higher level, but the SNR nearly becomes to be unchanged in the high intensity region.

We therefore assume the simple relation between the standard deviation and the intensity as expressed in Eq. (1), implying that the standard deviation is proportional to the intensity and approaches to the noise floor at the lowest intensity signal region

$$\sigma_I(\omega) = C(I(\omega) - h) + h \tag{1}$$

where ω is angular frequency, $\sigma_I(\omega)$ is the standard deviation of the intensity, $I(\omega)$ is the mean intensity, h is the noise floor, and C is assumed as a proportionality constant. We calculated the values of C from the standard deviation and intensity spectra of reference and sample using Eq. (1) to verify its validity. Fig. 2 shows the values of C decrease from the higher frequency to lower frequency, meaning that SNR is improved, and increase a little below 1 THz, implying the SNR becomes worse though the intensity still increases there. These facts suggest that the SNR is almost unchanged around the high intensity region, and hence the standard deviation becomes explicitly proportional to the intensity and C can be taken as a constant independent from frequency. Eq. (1) provides the simplest computational model using the constant C to derive the standard deviation from the intensity spectrum. The value of C does not depend on samples, since it is common in the reference and sample as shown in Fig. 2. Therefore, it can be determined by the intensity and standard deviation spectrum of only the reference in the high

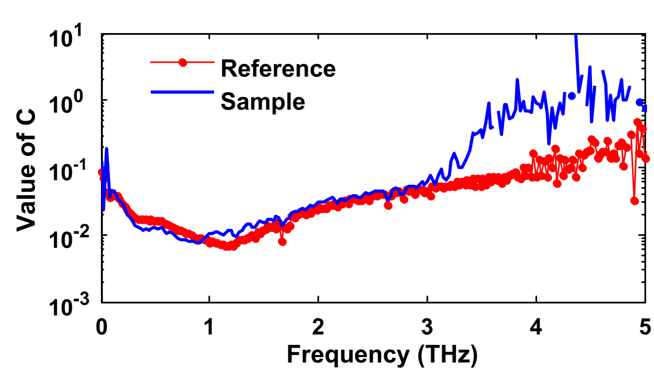

Fig. 2. Values of C calculated at various frequencies from the intensities and standard deviations of reference and the 0.767 mm-thick ZnTe sample using Eq. (1).