Optimization of Material Thickness for THz-TDS

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Abstract—**How thick should a sample be for a transmission-mode THz-TDS measurement? Should a sample be as thick as possible? The answer is 'no'. Although greater thickness allows T-rays to interact more with bulk material, the SNR rolls off with thickness due to signal attenuation. So, should a sample be extremely thin? Again, the answer is 'no'. A sample that is too thin renders itself nearly invisible to T-rays, in such a way that the system can hardly sense the difference between the sample and a free space path. Hence, where is the optimal boundary between 'too thick' and 'too thin'? The analytical expression to find the optimum thickness is revealed in this paper. This optimality results in the minimal uncertainty of measured optical constants. The derived model for optimal thickness is supported by the results from experiments performed with polyvinyl chloride (PVC) and other materials.**

I. INTRODUCTION AND BACKGROUND

It is well known to every THz-TDS experimentalist that, in transmission-mode spectroscopy, a sample that is too thick has considerable bulk absorption and can significantly reduce the signal power. Therefore, a sample is usually made very thin as long as it can be mechanically supported. However, a sample that is too thin can also cause problems, as the system might not be sufficiently sensitive to detect resultant changes in the amplitude and phase of the signal. Both thickness extremes result in higher uncertainty in the measured optical constants. In this paper, the optimal trade-off between the two extremes is determined, to minimize the uncertainty in optical constants.

II. UNCERTAINTY IN OPTICAL CONSTANTS

Given that the sample under a transmission-mode measurement has parallel and polished surfaces, and the angle of incidence of the incoming T-ray beam is normal to the surfaces, the transfer function of the sample is expressed as

$$H(\omega) = E_{\text{sam}}(\omega)/E_{\text{ref}}(\omega)$$
$$= \tau\tau' \exp\left\{-\kappa(\omega)\frac{\omega l}{c}\right\} \exp\left\{-j[n(\omega) - n_0]\frac{\omega l}{c}\right\}, \quad (1)$$

where $E_{\text{ref}}(\omega)$ and $E_{\text{sam}}(\omega)$ are the reference and sample signals in the frequency domain; l is the sample thickness; $n(\omega)$ and $\kappa(\omega)$ are the refractive index and the extinction coefficient of the sample; n_0 is the refractive index of air; and τ and τ' are the transmission coefficients at the sample interfaces. The refractive index and the extinction coefficient can be deduced from Eq. 1 as

$$n(\omega) = n_0 - \frac{c}{\omega l}\angle H(\omega), \quad (2a)$$

$$\kappa(\omega) = \frac{c}{\omega l}\{\ln|\tau\tau'| - \ln|H(\omega)|\}. \quad (2b)$$

Influenced by the variance in measured signals, the variances in the refractive index, $s_n^2(\omega)$, and in the extinction coefficient, $s_\kappa^2(\omega)$, can be derived from Eq. 2 using the law of propagation of uncertainty. In brief, from the signal amplitudes in the time domain, the variance is transferred to the variance of the magnitude and phase spectra in the frequency domain via Fourier transform. Then the combination between the variances of sample and reference measurements produces the variance in the transfer function of a sample. The variance eventually appears at the optical constants. From this analysis, the variances in the refractive index and in the extinction coefficient are given by, respectively,

$$s_n^2(\omega) = \left(\frac{c}{\omega l}\right)^2 \left\{\frac{A_{\text{sam}}(\omega)}{|E_{\text{sam}}(\omega)|^4} + \frac{A_{\text{ref}}(\omega)}{|E_{\text{ref}}(\omega)|^4}\right\}, \quad (3a)$$

$$s_\kappa^2(\omega) = \left(\frac{c}{\omega l}\right)^2 \left\{\frac{B_{\text{sam}}(\omega)}{|E_{\text{sam}}(\omega)|^4} + \frac{B_{\text{ref}}(\omega)}{|E_{\text{ref}}(\omega)|^4} + \left(\frac{n(\omega) - n_0}{n(\omega) + n_0}\right)^2 \frac{s_n^2(\omega)}{n^2(\omega)}\right\}, \quad (3b)$$

where

$$A_{\text{sam}}(\omega) = \sum_k \Im^2[E_{\text{sam}}(\omega)\exp(j\omega k\Delta)]s_{E_{\text{sam}}}^2(k), \quad (4a)$$

$$A_{\text{ref}}(\omega) = \sum_k \Im^2[E_{\text{ref}}(\omega)\exp(j\omega k\Delta)]s_{E_{\text{ref}}}^2(k), \quad (4b)$$

$$B_{\text{sam}}(\omega) = \sum_k \Re^2[E_{\text{sam}}(\omega)\exp(j\omega k\Delta)]s_{E_{\text{sam}}}^2(k), \quad (4c)$$

$$B_{\text{ref}}(\omega) = \sum_k \Re^2[E_{\text{ref}}(\omega)\exp(j\omega k\Delta)]s_{E_{\text{ref}}}^2(k). \quad (4d)$$

Here, $s_{E_{\text{ref}}}^2(k)$ and $s_{E_{\text{sam}}}^2(k)$ are the variances associated with the reference and sample signals, respectively; k is the sampling index number and Δ is the sampling interval, and thus $k\Delta$ is the time; $\Re^2$ and $\Im^2$ denote the square of real and imaginary parts, respectively. The summation is carried out over the time duration of the recorded T-ray signal. In the equations, all parameters utilize mean values. The proposed model in Eq. 3 is successfully validated with Monte Carlo method. A complete derivation for Eq. (3) can be found in [1].

III. OPTIMIZATION OF THE SAMPLE THICKNESS

In Eq. 3a, $E_{\text{sam}}(\omega)$ can be expressed in terms of $E_{\text{ref}}(\omega)$, and thus Eq. 3a is rearranged to

$$s_n^2(\omega) = \frac{C}{l^2}\left\{\frac{A'_{\text{sam}}(\omega)}{\exp(-4\kappa\omega l/c)} + A_{\text{ref}}(\omega)\right\}, \quad (5)$$

where $C = c^2/\{\omega^2|E_{\mathrm{ref}}(\omega)|^4\}$; $A'_{\mathrm{sam}}(\omega) = A_{\mathrm{sam}}(\omega)/(\tau\tau')^4$. By minimizing Eq. (5) with respect to the thickness l we obtain the optimum thickness,

$$l_{\mathrm{opt}} = \frac{c}{\omega\kappa(\omega)} = \frac{2}{\alpha(\omega)}. \tag{6}$$

A sample with optimum thickness attenuates the magnitude of the incident pulse by the factor of $1/e$. The optimum thickness turns out to be a distance that is equal to twice the penetration depth. Optimization of the sample thickness by starting from Eq. 3a also delivers the same outcome. A complete derivation for Eq. 6 can be found in [2].

IV. RESULTS

The measurement is carried out with normal-grade PVC, which is preformed in a rod shape. The rod with a diameter of 50 mm is cut into four cylindrical segments, with the thickness of 1, 10, 20, and 50 mm. The surfaces of these samples are well polished to minimize scattering. Each sample is measured with a collimated beam from the THz-TDS system in the axial direction for ten scans, and each scan is made after the previous scan within 30 s.

The optimum thickness for PVC, which supposedly yields the lowest variance in the measured optical constants, is determined from the absorption coefficient using the proposed model in Eq. 6. Fig. 1 illustrates the optimum thickness determined directly from the measured coefficient and from the fitting model. It can be seen that at frequencies around 1.0 THz, a sample thickness of 1 mm would provide the lowest variance of the optical constants. In addition, at low frequencies the optimum thickness increases by around one order of magnitude.

Fig. 2 shows the standard deviations of the optical constants for the four PVC samples, in terms of the unprocessed scatter plots and the fitting parametric curves. It is evident that at 0.05-0.2 THz, the 50-mm-thick sample provides the lowest standard deviation among the four samples; at 0.2-0.25 THz, the 20-mm-thick sample; at 0.25-0.6 THz, the 10-mm-thick sample; and above 0.6 THz, the 1-mm-thick sample. This optimum relation is in perfect agreement with the prediction in Fig. 1, which is derived using our optimal-thickness model. The improvement in measurement accuracy can be observed, for example, by comparing the standard deviations of the 1-mm-thick and 50-mm-thick sample. At around 0.1 THz the standard deviation for the thicker sample is $\approx 4\times10^{-5}$ and that for the thinner sample is $\approx 2\times10^{-3}$, or the improvement of the standard deviation is by almost two orders of magnitude.

V. USAGE OF THE MODEL

When selecting the optimum thickness, two options are available: (i) have the widest measurement bandwidth, or (ii) have the lowest uncertainty at a particular frequency. If the widest bandwidth is required, the maximum absorption value within the reliable frequency range of the system should be used in determination of the optimum thickness. This results in a thinner sample thickness thus retaining the bandwidth of the system and avoids dynamic range limited distortion, while

providing a reasonably low uncertainty in the measurement. There is a possibility that one might need to observe a sample's response in a narrow frequency range, with the highest precision available from the instrument, for example, in order to resolve a weak absorption peak hidden beneath the noise or to quantify the ratio of a mixture. In such cases, the optimum thickness calculated at the frequency of interest is indeed the best selection.
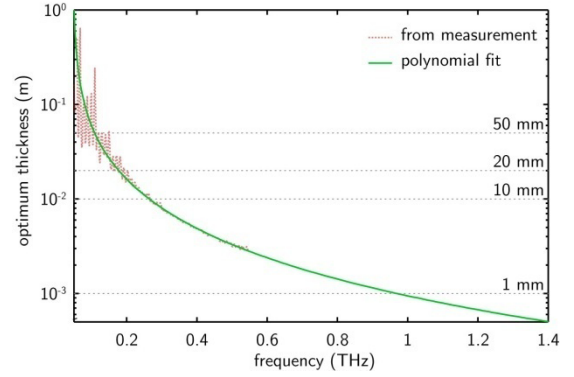

Figure 1. Optimum thickness for PVC. The solid line is a second-order polynomial fit to the absorption coefficient between 0.05 and 0.55 THz.
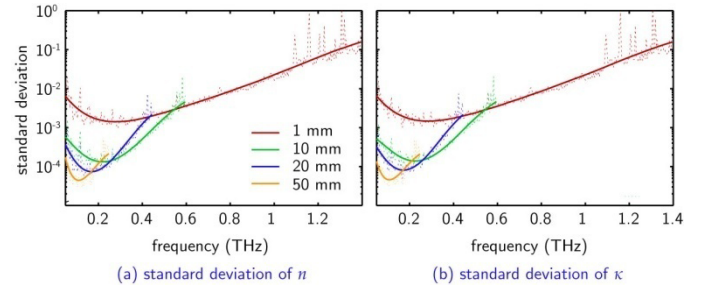

Figure 2. Standard deviations in the optical constants of PVC. Each standard deviation is determined from ten reference and ten sample signals. The missing part of the profiles in the high frequency range corresponds to the low SNR portion of the measured spectra.

VI. CONCLUSION

This work offers a criterion in selecting the optimum thickness of a sample. Provided that the absorption of a sample material at a frequency of interest can be estimated or approximated, the proposed model can predict the optimum thickness, which gives the lowest uncertainty in measurement. The derivation of the criterion is carried out via minimizing the uncertainty in optical constants—in terms of the variance or standard deviation—which is affected by the variance in measured time-resolved signals. The model is validated with a number of samples. More experiments can be found in [2].

REFERENCES

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