Mitigating Scattering Effects in THz-TDS Measurements

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Abstract—Scattering is a major problem in precise measurement of quasi-optical parameters of material samples. In this paper, we review some popular scattering mitigating techniques and propose a novel method that allows calculating true absorption spectra for samples with unknown thickness and granularity.

I. INTRODUCTION
At a fundamental level, the interaction of terahertz rays with materials with random structure is not completely understood at present. Scattering is a major problem for studying polycrystalline material samples at THz frequencies. When the size of scattering centers becomes comparable to THz wavelengths, the scattering process becomes rather complex and cannot be adequately explained by a simple Rayleigh model. Another area of concern is the dependence of scattering effects on the sample thickness. As the sample thickness is increased, the incident pulse has to travel a longer distance through the sample and so interacts with a larger number of scattering centers, thus suffering a greater degree of scattering. While under laboratory conditions, it is relatively straightforward to determine sample thickness and use it in the calculation of quasi-optical parameters; in real world applications, this is often impractical, e.g. in security.

Various researchers have contributed to resolving the issues surrounding scattering. One of the simplest and most popular techniques for reducing scattering effects in a granulated sample with large particle sizes (diameter 53 to 800 μm) is time averaging over multiple points, introduced by Shen et al. [1]. In this technique the sample is irradiated with THz radiation at different points on its surface and the resulting output THz pulses are averaged over time. However, since this technique relies on knowledge of thickness and sample particle size, it is only reliable for laboratory experiments. Another way to mitigate the effects of scattering is to window the radiation detected at the detector, such that the system will not detect any late arriving photons due to the etalon effect. This simple approach discards potentially useful measurement samples and it may lose critical spectral resolution.

II. METHOD DETAILS
In this paper we introduce a technique that can overcome the above described limitations and allows the calculation of the true absorption spectra for unknown sample thickness and granularity of the samples. We consider a monochromatic plane wave of frequency ω propagating through a material with complex dielectric constant $\tilde{n} = n + ik$ in z direction. The time dependent electric field can be expressed as:

$$E(z, t) = E_0 \exp \left\{ i \left( \omega t + \frac{\tilde{n} \omega}{c} z \right) \right\}$$  (1)

Consider this wave travelling through two different thicknesses $d_1$ and $d_2$ ($d_2 > d_1$) of samples of the above described material. In frequency domain the ratio of sample magnitude responses can be written as:

$$\frac{T_{s1s2}}{T_{s2s2}} = \exp \left\{ -\frac{k_4(\omega)c}{d_1} \right\}$$  (2)

or after simple manipulations, we can write

$$\log (T_{s1s2}) = \frac{\omega}{c} \{ k_2(\omega)d_2 - k_4(\omega)d_1 \}$$  (3)

In the above equation, $k(\omega)$ the extinction index is related to the absorption index $\alpha'(\omega)$ as:

$$\alpha'(\omega) = 2k(\omega) \frac{\omega}{c}$$  (4)

Now this absorption index $\alpha'(\omega)$, which represents the total loss suffered by the radiation, can be split in two components, absorption loss $\alpha_{ab}(\omega)$ and scattering loss $\alpha_s(\omega)$ as expressed in [2]:

$$\alpha'(\omega) = \alpha_{ab}(\omega) + \alpha_s(\omega)$$  (5)

Using equation (4) and (5), we can rewrite equation (3) as:

$$2\log (T_{s1s2}) = \{ \alpha_{2ab}(\omega)d_2 - \alpha_{1ab}(\omega)d_1 + \alpha_{2s}(\omega)d_2 - \alpha_{1s}(\omega)d_1 \}.$$  (6)

As all the material properties for the two samples are identical, we expect the “fingerprint” absorption features to be present at the same frequency bins. However, as the thicknesses of the samples are different, the amplitude of the absorptive features will be different. Therefore, in equation (6), the term $\alpha_{2ab}(\omega)d_2 - \alpha_{1ab}(\omega)d_1$ tends to cancel out the absorption features of the material leaving only a small remainder, which can be removed by smoothing the whole $\log (T_{s1s2})$ curve.

Therefore it can be assumed that in equation (6), the contribution of the term $\alpha_{2ab}(\omega)d_2 - \alpha_{1ab}(\omega)d_1$ is negligible or 0. Thus we are left with:

$$2\tau (\log (T_{s1s2})) = \{ \alpha_{2s}(\omega)d_2 - \alpha_{1s}(\omega)d_1 \}$$  (7)

where $\tau$ is the smoothing parameter.

Here we make another assumption that the sample thickness $d_1$ is such that this sample produces sharp absorption features with negligible scattering loss. Therefore, the scattering
contribution $\alpha_{15}(\omega)$ of sample 1 pulse is assumed to be zero. Then equation (7) can be expressed in terms of $\alpha_{2s}(\omega)$ as:

$$\alpha_{2s}(\omega) = 2 \cdot A \cdot \tau (\log (T_{2s1s}))$$  \hspace{1cm} (8)

where $A = \frac{1}{d^2}$. Therefore the true absorption spectra for the second sample can be determined by:

$$\alpha_{2ab}(\omega) = \alpha_2(\omega) - 2 \cdot A \cdot \tau (\log (T_{2s1s}))$$  \hspace{1cm} (9)

As the thickness of the samples is unknown, the parameter $A$ needs to be estimated or calculated iteratively to produce minimum baseline slope in the spectra of $\alpha_{2ab}(\omega)$.

III. SCATTERING CORRECTION

This approach uses the concept of generation of echoes due to the multiple reflections of a THz pulse while travelling through a thick sample. In the case of an optically thick sample, the echoes can be easily separated in the time domain. In our approach, we will only consider the first echo. Since the echo travels further in the sample as compared to the main transmitted pulse, it interacts with a greater number of scattering centres and therefore suffers more scattering. Therefore instead of using two different samples, we use these two pulses to obtain the required scattering estimate.

1. Simple scattering subtraction:

This method is essentially an implementation of equation (9) as described in the previous section. Once the parameter $A$ is estimated after a few iterations, the scattering estimate thus obtained can be simply subtracted from the original extinction spectra to obtain reasonable absorption spectra for a given material. This can be seen in Figure 1.

2. Filter based scattering correction:

The idea behind this technique is to design a discrete time filter that acts as a scattering cancelling device. That is, the required filter takes a scattered time domain signal as input and produces a scattering reduced time domain signal at the output. This can be done by designing a FIR filter using the frequency sampling method where the desired magnitude of the frequency response is specified by the inverse of the scattering estimate as obtained in equation (8) of the previous section, assuming the parameter $A$ is 1. The order of the filter is estimated iteratively, to produce minimum baseline slope for the absorption spectra obtained using the filter output. Thus when a scattered pulse is fed to the filter, it cancels out significant amount of scattering from the pulse to produce a less scattered version of the input signal, which can be further used to calculate the true or improved absorption spectra as shown in Figure 2.

![Figure 1. Extinction spectrum of alpha-glucose and P.E. pressed pellet samples (using THz TDS spectroscopy) with estimated scattering and scattering subtracted extinction spectra. Note: "fingerprint" features for glucose are ideally present at 1.455, 2.1, 2.6 and 2.78 THz [3].](image1)

Figure 1 clearly shows a significant improvement in the observed absorption features at around 1.45, 2.1 THz and slight improvement at 2.6 THz absorption feature, and a clear reduction in the slope of the baseline owing to the scattering posed by the sample.

![Figure 2. Extinction spectrum of alpha-lactose and P.E. (1:3 ratio) pressed pellet samples (using THz TDS spectroscopy) with Filter based scattering corrected extinction spectrum. Note: “fingerprint” features for lactose are ideally present at 0.53, 1.2 and 1.37 THz [4].](image2)

Figure 2 clearly shows a significant improvement in the observed absorption features at around 1.37 THz, and a clear reduction in the slope of the baseline owing to the scattering posed by the sample.

In conclusion, we introduce a novel technique that utilises the usually discarded echoes generated during the THz - TDS transmission spectroscopy to estimate the scattering and determine the true absorption spectra of a sample with unknown thickness, granularity and refractive index.

REFERENCES