Scattering Estimation from Spectral Moments of THz-TDS Signals

Mayank Kaushik[a], Brian W.-H. Ng.[a], Bernd M Fischer[a,b] and Derek Abbott[a]
[a] School of Electrical and Electronic Engineering, The University of Adelaide, South Australia.
[b] Institut Franco-Allemand de Recherches de Saint Louis, 68301 Saint Louis Cedex, France

***Abstract*—Scattering poses a major challenge to the precise measurement of spectral parameters of various materials. In this paper, we propose a novel signal processing based method of estimating scattering loss of a medium without precise information of its granularity, refractive index, and density.**

I. Introduction and Background

Scattering is a limiting factor for studying spectral signatures of polycrystalline samples at THz frequencies. When the sizes of scattering centres become comparable to THz wavelengths, the scattering process becomes rather complex and cannot be adequately explained by a simple Rayleigh scattering model.

Several researchers have provided contributions in order to explain and understand the key issues surrounding scattering in the terahertz region. In 2008, Franz et al. [1] applied the Christiansen effect theory to explain the scattering observed in the THz time domain spectroscopy (THz-TDS) measurements of granular samples. Their scattering estimate was based on the theoretical description provided by Raman spectroscopy on the propagation of electromagnetic radiation in inhomogeneous media and required knowledge of frequency dependent refractive index of the material. On the other hand, in 2007, Zurk et al. [2] applied a dense medium model to calculate an effective wave number within the quasi-crystalline approximation (QCA) to study THz transmission through pressed pellets of granular polyethylene (PE) with varying grain sizes. Their QCA solution not only required knowledge of parameters such as particle size, bulk dielectric constant, and volume fraction of constituents, but also relied on assumptions like a spherical shape for particles, dense packing and known positions within the sample. In 2010, Kaushik et al. [3] introduced a new technique that used Fresnel echoes generated during the THz-TDS process to estimate and mitigate the scattering effects in the measured extinction spectrum of the sample under study. This technique relied on the availability of strong and time resolved Fresnel echoes for estimating the scattering loss.

In this paper we introduce a technique that can overcome the above described limitations and allows the estimation of scattering loss for unknown sample granularity, refractive index, and packing density of the media, which can be further utilized to mitigate scattering effects from the THz-TDS measurements.

II. Method Details and Results

When a plane wave of frequency f propagates through a material with complex dielectric constant, it suffers frequency dependent attenuation because of absorption and scattering from the material. Both losses are frequency dependent, but the pattern of frequency dependence differs markedly from each other. Generally, scattering depends on the dimensions and density of the internal structure of the media, and this dependence can be expressed as a linear or quadratic over the given frequency range [4]. In contrast, absorption is a consequence of intermolecular vibrations in the media and for materials that exhibit sharp absorption features, such as α-monohydrate lactose, are confined to distinct frequency bins specfic to the constituents of the media, and therefore we assume that sharp absorption features can be expressed as higher order polynomials over the frequency range.

In our proposed approach, we consider a plane wave of frequency f propagating through a sample of material with complex dielectric constant, with thickness d. The Fourier transform of the transmitted signal is given by:

$$Y(f) = X(f)e^{i\varphi(f)}e^{-\alpha(f)d}, \tag{1}$$

where $X(f)$ is the Fourier transform of the signal before propagating through the sample, $\varphi(f)$ represents the phase shift and $\alpha(f)$ represents the total attenuation suffered by the signal.

In this paper, we explore the relation between the change in spectral moments of a THz pulse when it passes through a sample material and the frequency dependent scattering loss that occurs as a result of the interaction of the THz radiation with the internal structure of the sample material. In order to do this, we have to assume an analytical expression to describe the THz signal. One popular analytical model for the terahertz signal generated and detected using photoconductive antennas was given by Duvillaret et al. [5]. Their expression depends mostly on the carrier lifetime in the antenna's semiconductor material and on the laser pulse duration. The general formula to find the moments of a spectrum $S(f)$ is given by:

$$m_{\mathrm{n}} = \frac{\int_0^\infty f^n S(f)df}{\int_0^\infty S(f)df}. \tag{2}$$

Unfortunately, this analytical model does not have a closed form solution for calculating the moments using the above equation. Thus in order to find a standard representation of the detected reference THz spectrum, we tried fitting various well known distributions to the measured spectrum and found Rayleigh distribution to be a very good match. The result of the fit can be seen in Fig. 1, and the goodness of fit parameters are tabulated in Table 1.

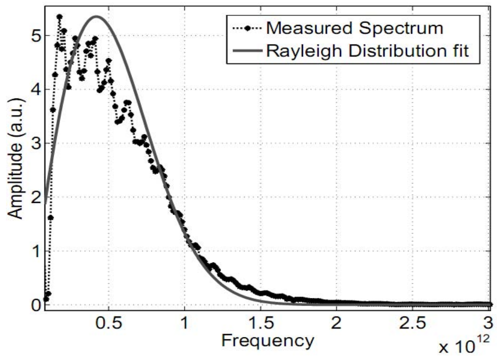

Figure1: Measured spectrum and Rayleigh distribution fit.

Thus, $|X(f)|$, the amplitude spectrum of the reference signal can represented as follows:

$$|X(f)| = A \frac{f}{\sigma^2} \exp\left(-\frac{f^2}{2\sigma^2}\right), \quad (3)$$

where, A represents the maximum amplitude of the T-ray field, f represents the frequency and σ is a distribution parameter.

Table 1: Goodness of fit: Measured spectrum and fitted Rayleigh distribution

Parameter	Value
Coefficient of Correlation	0.9645
Normalized MSE	0.0766

Now, using Eq. (2), we find the first order spectral moment (mean frequency of the spectrum) for $X(f)$ as:

$$\mu_{\mathrm{r}} = \sigma \sqrt{\frac{\pi}{2}} \approx 1.253\,\sigma. \quad (4)$$

When we introduce the sample to this system, the THz signal is attenuated from passing through the sample. For this analysis we consider only the materials that are transparent to THz frequency range and show no absorption features. Thus we can assume that the attenuation is completely due to scattering and can be expressed as a linear function of propagation length d and a quadratic over the given range of frequency. Thus, the amplitude spectrum of the sample THz signal can be given by:

$$|Y(f)| = A \frac{f}{\sigma^2} \exp\left(-\frac{f^2}{2\sigma^2}\right) \exp\left(-\alpha_s d f^2\right). \quad (5)$$

This further reduces to:

$$|Y(f)| = \frac{A}{(1+2\alpha_s d\sigma^2)} \frac{f(1+2\alpha_s d\sigma^2)}{\sigma^2} \exp\left(-\frac{f^2(1+2\alpha_s d\sigma^2)}{2\sigma^2}\right), \quad (6)$$

or

$$|Y(f)| = A' \frac{f}{{\sigma_s}^2} \exp\left(-\frac{f^2}{2{\sigma_s}^2}\right), \quad (7)$$

where, A' represents the maximum amplitude of the sample T-ray field, ${\sigma_{\mathrm{s}}}^2 = \sigma^2/(1+2\alpha_{\mathrm{s}} d\sigma^2)$, and the first moment for $|Y(f)|$ is given by replacing σ by σ_{s} in Eq.(4). It can be seen that the spectral shape of the attenuated pulse remains unchanged. However, the attenuation for the sample has changed the mean μ_{r} of the reference spectrum to μ_{s}, for the sample spectrum. Once the mean of the two measured spectra, reference and sample transmitted THz signal, are obtained from the above equations, the unknown scattering attenuation coefficient (α_{s}) can be calculated from the first order spectral moments of the measurements and the frequency dependent scattering loss can be determined as :

$$\alpha_{\mathrm{s\_loss}} = \frac{\sigma^2 - {\sigma_s}^2}{2\sigma^2 {\sigma_s}^2 d} f^2. \quad (9)$$

Using a standard THz transmission spectroscopy setup, we carry out transmission measurements for two samples. The samples comprised of PE particles (average particle diameter 60 µm and 360 µm) contained in a sample holder made of the Cyclic Olefin Copolymer (Topas - Refractive Index 1.6) of dimensions 5 mm inner thickness and 1 cm diameter. As PE is transparent to T-rays in the frequency range of 0.1 THz to 1.6 THz, it shows no absorption features and the measured attenuation loss is entirely due to the scattering of the T-ray signal for the internal structure of the sample. For each sample, we compare the measured attenuation loss, with the estimated scattering loss given by Eq. (9). The results are depicted in Fig. 2:

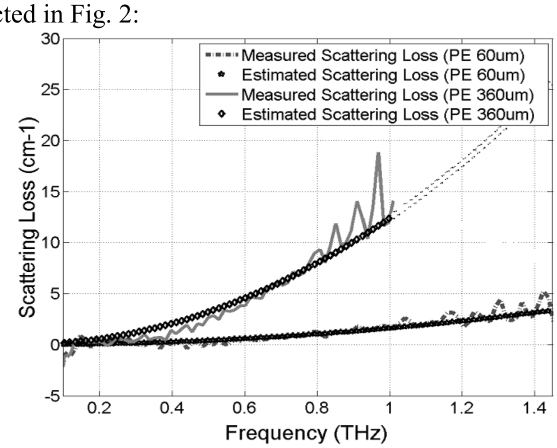

Figure 2: Extinction spectra of two different PE grain size with their respective estimated scattering loss profile.

III. CONCLUSION

As seen in Fig. 2, the technique reasonably estimates scattering loss profile for both the cases without using any *a priori* information of the physical characteristic of the sample or the material.

REFERENCES

[1] M. Franz, B. M. Fischer, and M. Walther, "The Christiansen effect in terahertz time-domain spectra of coarse grained powders," Appl. Phys. Lett. , 92, 021107 (2008).

[2] L. M. Zurk, B. Orlowski, D. P. Winebrenner, E. I. Thorsos, M. R. Leahy-Hoppa, and L. M. Hayden, "Terahertz scattering from granular material," J. Opt. Soc. Am. B 24, 2238−2243 (2007).

[3] M. Kaushik, B.W.-H. Ng, B. M. Fischer, and D. Abbott, "Mitigating scattering effects in THz-TDS measurements," 35th International Conference on Infrared, Millimeter and Terahertz Waves, (2010) doi: 10.1109/ICIMW.2010.5612470.

[4] K. A. Dines and A. C. Kak, "Ultrasonic attenuation tomography of soft tissues," Ultrasonic Imaging 1, 16−33 (1979).

[5] L. Duvillaret, F. Garet, J. -F. Roux and J.-L. Coutaz, "Analytical modeling and optimization of terahertz time-domain spectroscopy experiments, using photo-switches as antennas," IEEE Journal of Selected Topics in Quantum Electronics 7, 615−623 (2001).