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Time-Frequency Extraction of Sample Thickness and Spectroscopic Parameters using THz TDS

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***Abstract*—A new method allowing the extraction of both the thickness and complex refractive index of a sample simultaneously is demonstrated; the technique uses a time-segmented transfer function and model. Results are compared to an existing method of extraction.**

I. Introduction

TERAHERTZ time domain spectroscopy in transmission geometries has previously been demonstrated to be capable of extracting both the thickness, l, and complex refractive index, $\tilde{n}$, of a sample [1]. This has however relied on minimising etalon errors in the extracted values of $\tilde{n}$ to extract l, a process which can leave residual etalons in $\tilde{n}$. A new method, using a time segmented sample transfer function and model, to extract etalon free $\tilde{n}$ and l of a sample simultaneously is presented in this work.

II. Method

The sample transfer function is segmented across multiple time windows, such that each segment contains individual pulses generated by resonance within the sample. Models for each segment are fitted simultaneously at each discrete frequency, allowing us to extract both a sample's $\tilde{n}$ and l in a single extraction.

To segment the transfer function, H, into multiple time localised segments, H_δ, the transfer function of a sample is first calculated using a reference (dry air) and a sample measurement (which includes sample reflection pulses). H is then converted to the impulse response using an inverse Fourier transform. This impulse response will contain pulses which correspond to the initial transmission and following reflections from the sample. These pulses are individually windowed, and then Fourier transformed, to form different time segmented transfer functions, H_δ, where δ is the pulse index ($\delta = 0$ for initial pulse). In this work, only the first two pulses are used. We note that, while it is possible to fit using a larger number of pulses, this does not provide a significant advantage in terms of extracting either l or $\tilde{n}$, as phase information from other pulses will not provide any new information relating to either of these parameters.

To do this we have included a Gouy phase shift correction into the model [2] which includes a calibration parameter, β. β can be estimated from two different approximations of real refractive index, n, made from the initial pulse and first reflection of a calibration sample, with known sample thickness:

$$\beta = \frac{3}{2}\left(n_0 - n_1\right) \tag{1}$$

Where n_0 and n_1 are the real refractive index calculated from the initial and reflection pulses respectively. These are formed without accounting for the Gouy phase shift incurred by the sample displacing the focal point of the beam. As the path length is different for the initial transmission and first reflection, so will be the systematic error which can be used to calculate β. These can be calculated using the equation:

$$n_\delta = \frac{1}{2\delta + 1}\left(\frac{-c}{\omega l}\angle H_\delta + 1\right) \tag{2}$$

Where δ is the pulse index, c is the free space velocity of light, ω is angular frequency and $\angle H_\delta$ is the measured unwrapped transfer function phase for pulse δ.

Similarly, when measuring a sample, the pulse train can be segmented, leading to M segmented transfer functions, H_δ, for each pulse. $\tilde{n}$ and l can then be extracted at each frequency by minimising the sum of squared errors between H_δ and the transfer function pulse models, $\bar{H}_\delta$:

$$\tilde{n}(\omega), l(\omega) = \underset{\tilde{n},l}{\operatorname{argmin}} \sum_{\delta=0}^{M-1} \Big(\big(|H_\delta| - |\bar{H}_\delta(\omega, \tilde{n}, l)| \big)^2 + \big(\angle H_\delta - \angle \bar{H}_\delta(\omega, \tilde{n}, l) \big)^2 \Big) \tag{3}$$

By fitting the model of each pulse to a different transfer function segment, both the thickness and refractive index can be extracted simultaneously. By separating the pulses using segmentation, no etalons are present in any of the individual transfer function segments, and thus, no etalons can propagate into the final estimate of $\tilde{n}$.

A Gouy phase shift corrected sample transfer function pulse model, $\bar{H}_\delta$, is required to extract both $\tilde{n}$ and l simultaneously. Without using this correction, it is not possible to extract a constant measurement of thickness. Two coefficients for the Gouy phase shift correction were introduced, first an amplitude correction coefficient:

$$W_\delta = \frac{1}{\sqrt{1 + \left(\frac{\omega \beta l'_\delta}{c}\right)^2}} \tag{4}$$

Secondly, a phase correction coefficient:

$$G_\delta = e^{+i\frac{\omega \beta l'_\delta}{c}} \tag{5}$$

Both of which are a function of normalised propagation length through the sample, l'_δ, which for pulse δ is:

$$l'_\delta = (2\delta + 1)\frac{l}{n} - l \tag{6}$$

Where n is the real part of $\tilde{n}$.

The sample pulse transfer function model, $\bar{H}_\delta$, which models the pulse in each H_δ, is then:

$$\bar{H}_\delta = T_{a,s}T_{s,a}P_sP_a^{-1}R_{s,a}^{2\delta}P_s^{2\delta}W_\delta G_\delta \tag{7}$$

Where $T_{a,s}$ and $T_{s,a}$ are the transmission coefficients between the air and sample, and sample and air, respectively; P_a is the propagation coefficient of air over sample thickness l; P_s is the propagation coefficient of the sample; and $R_{s,a}$ is the reflection coefficient between the sample and air. These coefficients are defined in [1].

We compare this technique to a previously established technique of extracting a sample's parameters, and show that this method provides an accurate measurement of l and etalon free values of $\tilde{n}$.

III. Results

A 0.512 mm z-cut quartz sample was measured, using a transmission THz time domain spectrometer described in [3], with LT-GaAs-on-quartz based emitters and detectors described in [4]. β was estimated from a 0.58 mm high resistivity silicon plate. In Figure 1, the estimated n_0 (blue) and n_1 (green) of the calibration silicon are shown. Using the difference, β can be estimated (dashed blue line). As the estimate is susceptible to noise, a smoothed estimate was used (red line), made using a moving average function.

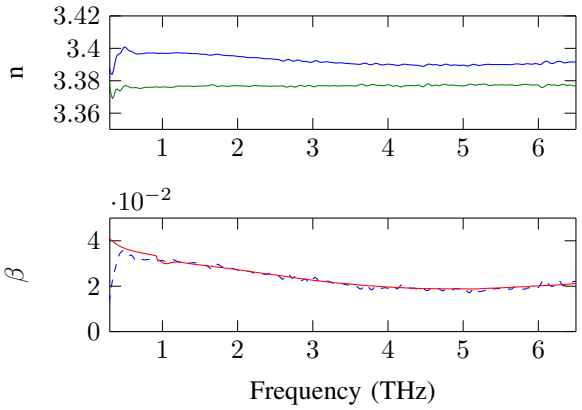

Fig. 1. Estimated values of n_0 (blue) and n_1 (green) for a 0.58 mm high resistivity plate. The estimated calibration coefficient, β, (blue dashed), with the smoothed estimate used for sample extraction (red).

In Figure 2, the extracted values of n, κ (extinction coefficient) and l of the quartz sample are shown. These values were extracted using different methods, using a resonant model with total variance for thickness extraction [1] (green), using the same method with a Gouy phase shift corrected model (blue) and using our time segmented model and transfer function (red). The uncalibrated estimate (green) of sample thickness was 0.503 mm, while the calibrated methods (blue and red), both gave (average) values of 0.515 mm. The quartz sample contains a resonant mode at 3.78 THz, which is partially obscured in the non-calibrated method. The estimates produce similar estimates of n and κ, with slight difference for extracted thickness, as well as etalons in the non-segmented methods. At frequencies below 1 THz, overestimation of the absorption occurs in the segmented method because of distortion during the segmentation. Further improvements to this technique could be made by improving the segmentation so that distortion is reduced.

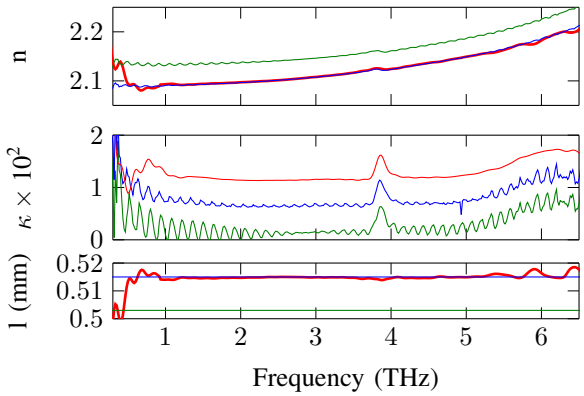

Fig. 2. Extracted values of n, κ (0.005 offsets) and l of a z-cut quartz sample.

IV. Conclusion

We have provided a new method of estimating a calibration coefficient, β, of a system using a single measurement of a calibration sample. This was then used to demonstrate a method of measuring sample thickness, l, and complex refractive index, $\tilde{n}$, of a sample using a time sensitive. This method was demonstrated to be as accurate as fitting a calibrated resonant model, but provides smoother estimates of $\tilde{n}$.

V. Acknowledgement

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