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Uncertainties estimation in THz-TDS experiments in transmittance, refractive index and spectroscopic parameters

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Abstract— Data processing is a key for the spreading of the THz-TDS systems to more analytical fields. However, till today no standard methods exist to extract error bar from standard measurements in TDS besides the transmission. We propose here a methodology to reply to this challenge.

Keywords—Time Domain Spectroscopy, data processing

I. INTRODUCTION

THz time domain spectroscopy (THz-TDS) is now in its third decade, having transformed from bulky and very expensive setups using rare femtosecond laser facilities of this time to compact, commercially available and financially accessible instruments. This progress mirrors the advancements in femtosecond laser technology, which are now readily available through fiber optics and are as small as an external drive. The logical consequence of these improvements is a spreading of the techniques across diverse fields, extending far beyond the initial research community.

Pioneering investigations focused on engineering [e.g., [1], physics [2], and physical chemistry [3]. Today, THz-TDS finds use in food science and agro-industry [[4]], pharmaceuticals [5], and industrial applications.

However, accurate quantification hinges on a rigorous understanding of uncertainties in the measurements. While early research focused on demonstrating capabilities, new quantitative applications necessitate a more rigorous and standardized approach to expressing signal-to-noise ratio and uncertainties [6]. Notably, seminal work by Duvillaret et al. explored noise and uncertainty analysis two decades ago [7, 8]. However, the maturity of modern systems necessitates a renewed focus on standardization.

In this presentation, we will detail our efforts to leverage the signal-to-noise ratio, as determined in our research, to quantify uncertainties associated with transmittance, complex refractive index, and ultimately, the parameters derived from a full spectroscopic fit of the recorded data [9].

II. METHODOLOGY

We propose to use a step-by-step methodology propagating the uncertainties from the one recorded on the time traces during the experiments, to the first spectral quantities as the transmission, to the losses and refractive indices to end with the physical parameters describing the samples.

To get the uncertainties on our accumulated time traces we estimated the covariance matrix from our time traces following [10] and the standard deviation from our corresponding spectrum.

The standard deviation on the transmission is calculated as in

$$\sigma(\tilde{T}) = \sigma\left(\frac{\tilde{E}_S}{\tilde{E}_R}\right) = \tilde{T} \left[\frac{\sigma(\tilde{E}_S)}{\tilde{E}_S} + \frac{\sigma(\tilde{E}_R)}{\tilde{E}_R} \right],$$

Where \tilde{T} is the transmission in the frequency space, \tilde{E}_S the spectrum of the sample and \tilde{E}_R the one of the reference. From there, one can derive the metric losses, and by neglecting the interfaces terms, and a very rough evaluation estimation of the imaginary part of the refractive index $\kappa_{R.E.}$ by dividing it by the thickness of the sample. The corresponding uncertainty writes:

$$\sigma(\kappa_{R.E.}) = \sigma\left(\frac{\ln(\tilde{T})c}{2\pi f}\right) = \frac{c}{2\pi f} \frac{\sigma(\tilde{T})}{\tilde{T}},$$

Where c is the speed of light t the thickness of the sample and f the frequency.

In most of the cases, a more meticulous estimate of the refractive index needed, requiring to go through an optimization algorithm. In this case, the way to estimate the uncertainties is to perform the second derivative (or Hessian matrix) of the objective function when it itself is normalized by the uncertainty on the recorded signal. We implemented this in our software `fit@tds` allowing to retrieve now not only the refractive index but its uncertainties.

III. RESULTS

To test our methodology, we performed experiments on a 1 mm thick Z-cut quartz wafer. We set it in the collimated beam of a Terasmart TDS from Menlo system and recorded 100, 36 ps long, time traces for the references and for the samples. Figure 1 depicts the rough estimation of the imaginary part of the refractive index superimposed with the retrieve one from the optimization, together with their uncertainties. Figure 2 show the real part of the refractive index.

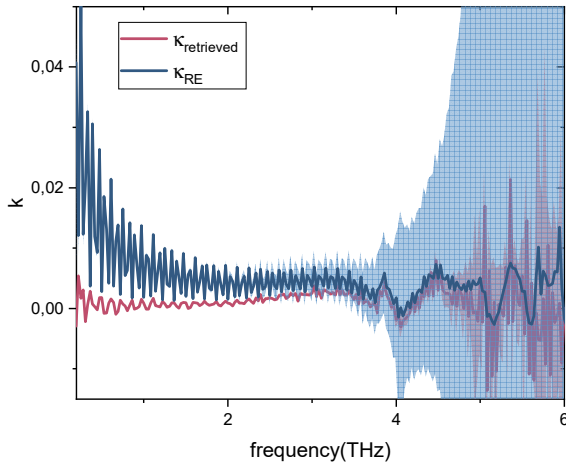


Figure 1 Imaginary part of the refractive index. Rough estimation and estimation of the uncertainties on it compared to retrieved value thanks to an optimization algorithm and corresponding uncertainties.

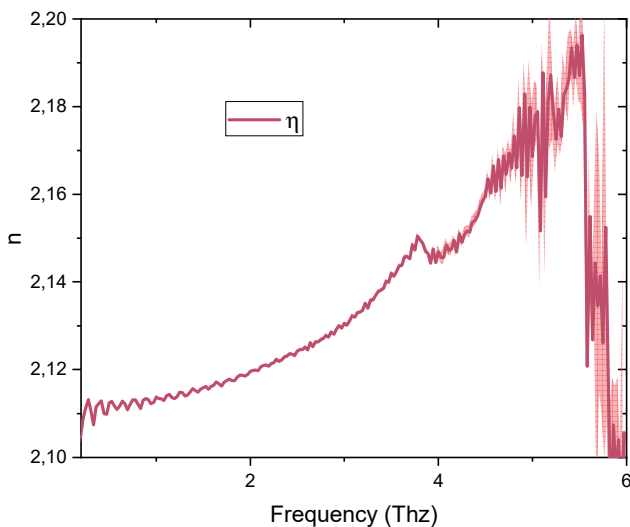


Figure 2 Real part of the refractive index retrieved value thanks to an optimization algorithm and corresponding uncertainties.

One can see on these figures that the uncertainties (plotted as 3 sigma) are very low compare to a visible oscillation in every spectrum. In fact, this oscillation corresponds to the Fabry Pérot oscillations giving two echoes in the time traces. This oscillation is taken into count in the retrieval algorithm as the two (an only two) echoes it gives, but this is not enough to remove the oscillation. In fact, the collimated beam probes the wafer on a surface with a diameter of about 38 mm, therefore the thickness of the sample is far from constant at

this precision and causes modification in the Fabry Perot leading to this oscillation.

IV. CONCLUSION

In the conference we will show how this effect is different while performing the experiments with a focus beam and how uncertainties on the thickness can be manage by a proper modelling of the system and fit the time traces

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