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From Noise analysis to Error Bars on Refractive Index In THz-TDS

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Abstract—We present a new methodology for computing error bars in THz-TDS experiments and distribute open source software for this purpose. Pursuing our efforts in noise analysis and data processing of THz-TDS experiments, we followed a standard approach to derive the error bars from the simplest quantities coming from the experiments (transmission, absorbance) and a Bayesian approach when using an optimization fitting methodology to retrieve the plotted magnitude (refractive indices).

I. INTRODUCTION

TIME domain spectroscopy (THz-TDS) is now in its third decade and grew from the bulky and very expensive setups of beginning using the rare femtosecond lasers of this time to very compact commercial and financially accessible apparatus. These progresses followed the ones of the femto-seconds lasers now available from optical fiber technology and as big as an external drive. The logical consequence of these developments is a spreading of the technics in many fields always further away from the initial community. Still today, the methods is not recognized as an analytical standard. We believe, with others [1], that one of the reason that THz-TDS did not take an even more important role in analytical field is the difficulty to derive uncertainties and error bars from the desired measured quantities.

In this conference, we will present how our efforts to fit the time trace of THz-TDS, and to analyze the noise of the systems [2, 3] brought us further away and enabled us to derive error bars in transmission and absorbance measurements first, and even while retrieving the complex refractive index of a sample.

II. RESULTS

To test our approach we performed experiments on the so-called golden sample, a pellet of pure alpha lactose monohydrate. This sample have been widely studied and is an excellent candidate for our objective since it includes frequency region of relatively low absorption while other contains strong absorption peaks impeding any signal to cross the pellet in their frequency region.

To extract uncertainties and errors bars from quantities of relevance for our sample we have first to record the uncertainties on our signal itself. As we already [4] explained elsewhere, and following the methodology proposed by [5, 6] we first get rid of several artifacts such as drift in temperature of the optical fiber leading to a delay in the data and estimate the noise by measuring the standard deviation of our signal during the experiments including 1000 accumulations. This methodology allows the estimation of the noise first in the standard deviation in the time domain but also in the

frequency domain.

Then using the frequency domain value for the uncertainties of the signal one can easily derive the one for a transmission measurements and with a little bit more of effort and assuming that the knowledge of the thickness of the sample does not add uncertainties one can derive the uncertainties on the absorbance as depicted on fig 1.

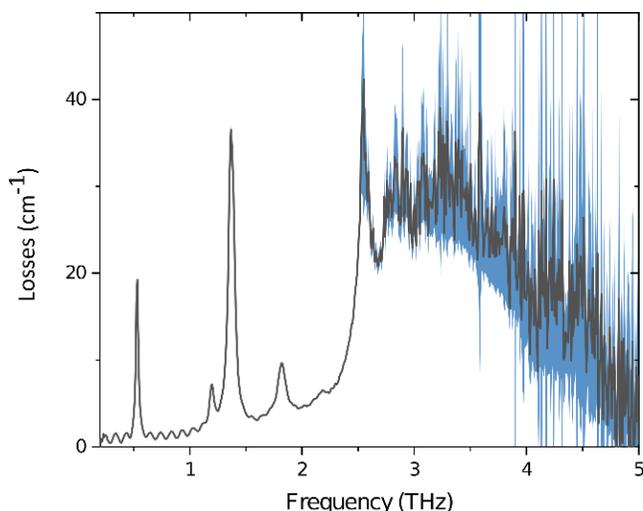


Fig. 1. In black curve, the usual losses (being the minus of the log of the transmittance) plotted versus frequency, in blue the variance derived from the one on the signal for the sample and the reference. A nice point with this plot is that the lowering of the losses between 2.5 and 3 THz are confirmed to be true and not an artifact.

Here one can see that the uncertainty on the loss is very small in the region of strong signal going to the receiver. Hence the hypothesis of neglecting the uncertainties due to the measurements of the thickness of the sample maybe broken in this region. In the more absorbing region, one can see an increase of the uncertainties while keeping reasonable values, due to the log in the loss formula.

To go a step further we decided to extract the complex refractive index from our sample. This problem is fully invertible when dealing with non-absorbing or relatively low absorbing sample but one needs to perform an optimization as soon as the imaginary part of the refractive index become non-negligible. Therefore getting uncertainties going through the optimization algorithm is one-step more complex. Here, we will use a Bayesian approach relating the uncertainties on the signal to the one on the retrieved n and k values by normalizing the error function in the fit routine by the noise. Hence, when the algorithm converges, the first derivative (gradient) is null and the variations are locally depicted by the second derivative (the Hessian). Using the normalization by the noise, the uncertainties on the retrieved value simply

become the diagonal terms of the inverse Hessian.

This is the methodology we used to plot the imaginary part of the complex index of refraction on fig 2.

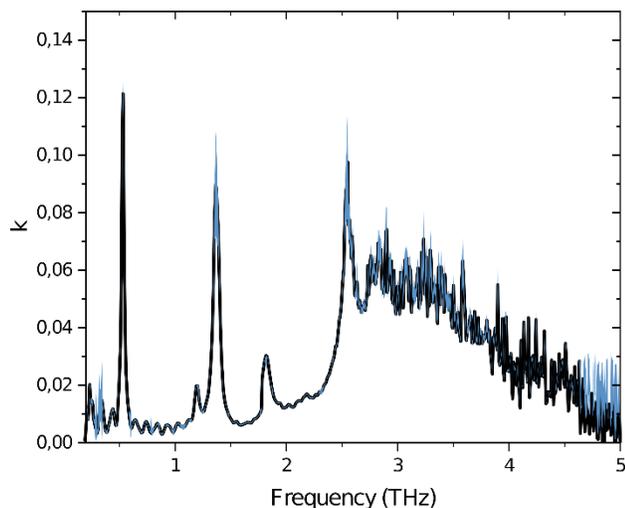


Fig. 2. Imaginary part of the complex refractive index in black, in blue the variance of it.

The variance goes from $1e-4$ around 1 THz to $1e-2$ around 3THz.

III. SUMMARY

In this conference, we will take the time to introduce how estimate the noise in THz-TDS experiments and propagate the uncertainties it introduces to the transmission, the transmittance, the refractive index and we hope that we will have reach the points of deriving the uncertainties of fitted magnitudes such as the central frequency or the width of a spectral lines.

We envision that these efforts will help to spread the technique to more analytical fields and become a new standard for myriads of applications.

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