

Time-domain data truncation method for improving terahertz absorption spectrum reproducibility

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Abstract—The confounding nature of the etalon-feature in THz frequency-domain spectra can be eliminated by truncating the time-domain data before the echoes. However, the spectra features are sensitive to the window length used to truncate the raw data. In this paper, we presented the impact of random truncation on the THz absorption features of L-Glutamine (Gln) and then put forward with an optimized time-domain data truncation (TDDT) method to improve the spectra reproducibility. Samples consist of Gln at three different concentrations were measured with THz-TDS to assess our method.

I. INTRODUCTION AND BACKGROUND

Spectroscopic applications utilizing THz-TDS provide useful chemical information of under-studied material. THz absorption features of solid-state sample related to overall vibration of crystalline, which paves way for noninvasive analysis of target sample combined with Beer-Lambert law. However, the analytical precision was limited by many factors by far. Those factors include accurate extraction of sample's thickness, migration of the baseline caused by scattering effect, proper preprocessing strategy for the raw time-domain data [1][2]. Efforts have been made for those challenges while our work focused on the truncation methods in preprocessing section.

In THz-TDS measurements, truncation of raw time-domain data prior to Fourier Transformation (FT) aims to remove the etalon artifacts in absorption spectra. Our study had proven that randomly windowing the data can introduce variations to absorption features and reduce the reproducibility of THz-TDS experiments. Thus a reliable method should be established to determine a proper truncation length for raw experimental data.

In this paper, we presented how the random truncation adversely impacts the absorption features calculated from a same set of experimental data of Gln. Then a method to determine the proper truncation position was proposed and experimentally assessed.

II. EXPERIMENTS

The sample we prepared were Gln (Wako Pure Chemical Industries, 078-05461) mixed with polyethylene for dilution. They were compressed together into tablets 13mm in diameter. Three samples consisted of Gln at different concentrations shown in Table. 1. Gln1 was designed to show how randomly truncation impacts the absorption spectrum and introduce the purpose of our truncation methods, the other two samples were designed to assess the reproducibility of our proposed method.

Sample Label	Gln1	Gln2	Gln3
Concentration (mol/L)	0.863	0.692	0.295
Thickness (mm)	1.20	0.81	1.32

All the samples were measured by transmission THz-TDS [3] at room temperature and in a vacuum box to avoid the influence of water vapor. The absorption coefficients were calculated as:

$$\alpha(\omega) = -\frac{2}{d} \ln \left[\frac{|E_{sam}(\omega)|}{|E_{ref}(\omega)|} \right]$$

where d is the thickness of sample. The truncation occurred before Fourier transforming the time-domain data $E_{sam}(t)$ and $E_{ref}(t)$ into $E_{sam}(\omega)$ and $E_{ref}(\omega)$.

III. IMPACTS OF RANDOM TRUNCATION

As shown in Fig. 1, different truncation (10ps, 12ps, 15ps) of the Gln1's experimental time-domain data gave rise to obvious artificial variations in corresponding absorption spectra, especially in high frequency range.

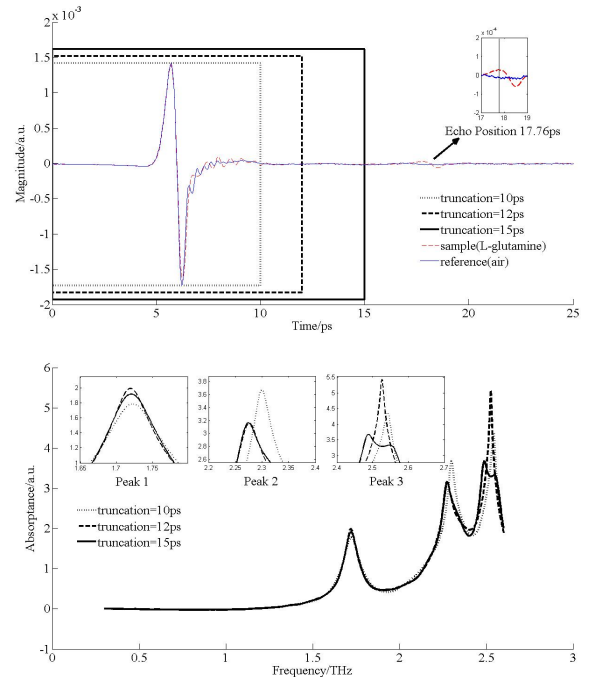


Fig. 1. The obvious variations in absorption spectra by truncating a same set of time-domain data before echoes at three different positions(10ps, 12ps, 15ps).

Table 1 Concentrations of L-Gln in three samples.

We speculated that the multiple-reflection of THz radiation inside the emitter semi-conductor material LT-GaAs should be responsible for this phenomenon. Because this reflection was recorded prior to the etalon-features caused by sample and it was not obvious to be truncated properly.

All the spectra with different truncation lengths varying from the end of main pulse t_0 to the beginning of the etalon-features t_N were plotted in Fig. 2. Although the spectra differed from each other, it was noticeable that they fluctuate in a certain region.

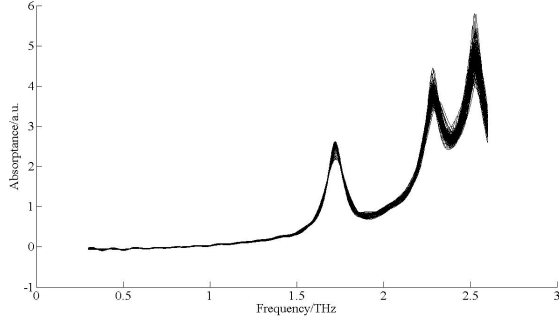


Fig. 2. All the spectra calculated from truncation length from the end of main pulse to the beginning of echo.

The purpose of our method was extract one absorption spectrum with a proper truncation length which could satisfy this overall pattern to characterize target material. We defined the optimized truncation position as $t_{truncation}$, which should minimize $s(t_i)$:

$$s(t_{truncation}) = \min \left\{ s(t_i) \mid s(t_i) = \sum_{\omega} \left[A(\omega, t_i) - \bar{A} \right]^2 \right\}$$

$$\bar{A} = \frac{\sum_{i=0}^N A(\omega, t_i)}{N + 1}$$

in which $A(\omega, t_i)$ is the absorption coefficient calculated with truncation position t_i .

IV. EXPERIMENTAL ASSESSMENT

We validated this truncation method in all the three pairs of experimental data. Best window lengths were listed in Table. 2 and the corresponding absorption spectra were presented in Fig. 3.

Table 2 Truncation positions of three samples determined by proposed method.

Sample	Gln1	Gln2	Gln3
Truncation position (ps)	13.5487	12.1633	13.6513

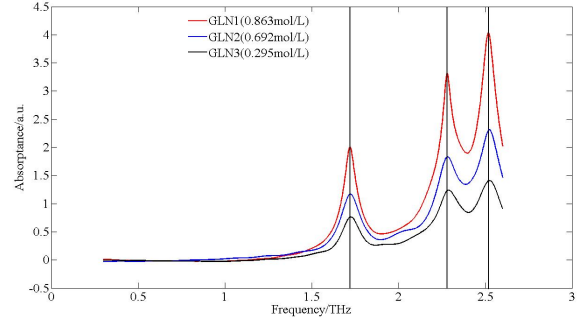


Fig. 3. The reproducibility of absorption features of Gln at three different concentrations with proper truncation position.

The spectra above showed that the three absorption features of Gln are stable without frequency shifts and capable for qualitatively identification, which indicated that our method is effective.

V. SUMMARY

In this paper, we presented the impact of random truncation on THz absorption spectra and introduced an optimized method for determining the proper truncation position in raw time-domain data. The validation of our method in three Gln samples at different concentration proved to be effective in improving the reproducibility of THz absorption spectra. Further study will focus on the relationship between this proper truncation length and experimental parameters like thickness and refraction index of sample.

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