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A method for removing etalon oscillations from THz time-domain spectra

M. Naftaly *, R.E. Miles

University of Leeds, School of Electronic and Electrical Engineering, Leeds LS2 9JT, United Kingdom

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Abstract

We present a simple algorithm for removing or reducing spurious oscillations in the THz spectra which result from secondary reflection peaks in samples or optical elements. The algorithm utilizes the fact that a THz time-domain trace containing secondary peaks can be represented as a convolution of the primary peak and two or more delta functions. The algorithm is applicable for samples which are sufficiently thick that the reflection peak does not overlap with the primary peak, and that do not have strong absorption or dispersion.

Keywords: THz time-domain spectroscopy; Spurious oscillations; Secondary reflections; Smoothing algorithm

1. Introduction

A well-known problem encountered in calculating terahertz absorption coefficients and refractive indices from data obtained by time-domain spectroscopy arises from spurious oscillations caused by the etalon effect in samples and optical components. In the time-domain data the presence of the etalon effect is manifested as secondary peaks following the primary THz peak. These may result from multiple reflections within samples, emitters or detectors [1,2]. When spectra are calculated from the time-domain data using Fourier transform (FT), these secondary peaks give rise to spurious etalon oscillations (Fig. 1), characterized by the frequency period of $1/\Delta t$, where Δt is the time difference between the primary THz peak and the secondary peak. Clearly, such oscillations interfere with data analysis and may obscure important features of the absorption spectrum.

Methods for removing secondary reflections in electro-optic detector crystals include anti-reflection coating [1] and combining two differently-oriented crystals [2]. However, there are no experimental techniques available for reducing secondary peaks originating in samples.

A simple and effective method for removing oscillations in the Fourier transform data is "adjacent averaging". In this, the ordinate value of each data point is replaced by the average value over a range centered on the target point. The oscillations are minimized when the averaging range is close to the oscillation period. This numerical technique is particularly suited to samples which exhibit a (monotonously) rising absorption edge lacking features. However, adjacent averaging is clearly inapplicable to spectra containing narrow peaks or other features because it effectively reduces frequency resolution. The same consideration also applies to truncating the data so as to exclude the reflection peak, because this also reduces frequency resolution.

Numerical data-analysis techniques have been developed which successfully remove etalon oscillations from the time-domain and/or frequency-domain data [3–6]. However, these often require iterative fitting procedures [3–5]; and always necessitate complex calculations. Although these methods are capable of producing highly accurate, low-noise data, they have not been widely adopted into use owing to the computational difficulties.

* Corresponding author.
E-mail address: M.Naftaly@leeds.ac.uk (M. Naftaly).

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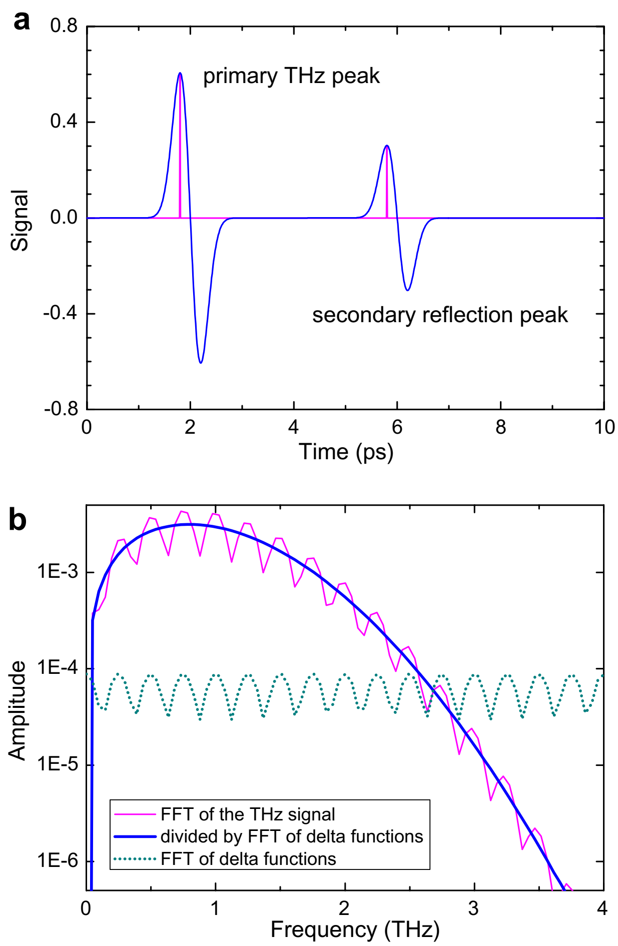

Fig. 1. An illustration, using model data, of the algorithm for the removal of spurious oscillations (the etalon effect): (a) The primary THz peak and the secondary peak, and the delta function set. (b) The FT spectrum of the THz signal; the FT of the THz signal divided by the FT of the delta function set; and the FT of the delta function set.

Here, we present a simple computational algorithm for removing, or at least reducing, spurious oscillations arising from the etalon effect. The main advantage of this technique over other numerical methods is its simplicity and ease of application. A further important benefit is that it does not reduce frequency resolution, thus leaving unaffected peaks and other features in the spectrum. The algorithm is applicable to time-domain data originating in samples which produce a secondary reflection peak (or several), but which are sufficiently thick that the secondary peak does not overlap with the primary peak. A limitation of the algorithm is that it is unsuitable for samples which are strongly absorbing and/or strongly dispersive.

2. The oscillation removing algorithm

The method relies on an approximation to the equation describing the propagation of pulsed electromagnetic waves through a Fabry–Perot etalon [7]. Accordingly, it utilizes the fact that a THz time-domain trace containing secondary reflection peaks may be approximated by a convolution of the primary THz peak and a set of delta functions corresponding to all the peaks in the trace:

$$A(t) = A_0(t) \times \sum_{i=0}^{\infty} a_i \delta(t_i) \tag{1}$$

where $A(t)$ is the time-dependent amplitude of the THz pulse, $A_0(t)$ is the amplitude of the primary peak, and a_i and t_i are respectively the amplitudes and time-domain positions of the secondary peaks; $i = 0$ refers to the primary pulse. The values of a_i and t_i can be obtained from the time-domain data by noting the maxima and time positions of all the peaks, as shown in Fig. 2.

The Convolution Theorem [8] states that the Fourier transform (FT) of a convolution of two functions is the product of their respective transforms. Therefore, the calculated spectrum $E(f)$ may be seen as a product of the true THz spectrum and the FT of the delta function set:

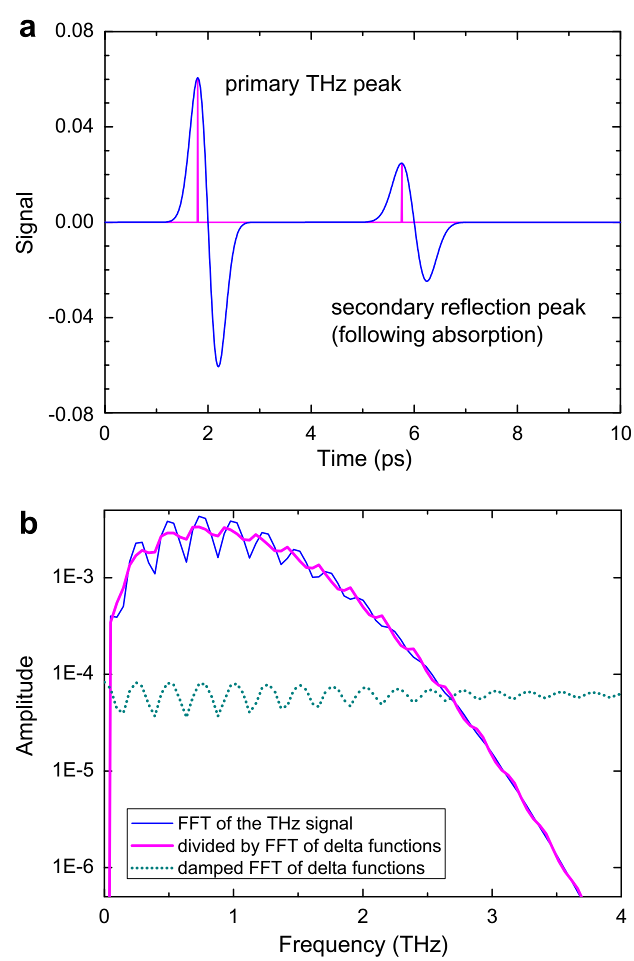

Fig. 2. An illustration, using model data, of the algorithm for the removal of spurious oscillations in the presence of absorption: (a) The primary THz peak and the secondary peak, and the delta function set. The secondary peak is broadened by absorption. (b) The FT spectrum of the THz signal; the FT of the THz signal divided by the modified FT of the delta function set; and the damped FT of the delta function set.

$$E(f) = \Im[A(t)] = \Im[A_0(t)] \times \Im\left[\sum_i a_i \delta(t_i)\right] \tag{2}$$

The second factor in the product in Eq. (2), i.e., the FT of the delta function set, can be calculated directly from the list of values of a_i and t_i. It must be remembered that the number of points and the step size in the delta function data set must be the same as in the primary trace. The correct THz spectrum may then be recovered by taking the ratio of the calculated source spectrum and the FT of the delta function set:

$$E_{\mathrm{true}}(f) = \Im[A_0(t)] = E(f) \times M/\Im\left[\sum_i a_i \delta(t_i)\right] \tag{3}$$

where M is the normalizing factor equal to the mean value of the FT of the delta set. This process is illustrated in Fig. 1 using model data. The normalizing factor M is necessary because the values of a_i in Eq. (1) are taken as the heights of the peaks in the time-domain trace, with a_0 being that of the primary peak. Alternatively, the values of a_i may be normalized so that $a_0 = 1$, with $a_{i>1}$ scaled appropriately, in which case $M = 1$ and is therefore redundant.

An additional difficulty arises when measuring THz transmission in absorbing materials. The great majority of such materials have absorption which increases with frequency. When that is the case the spectrum of the secondary peak is narrower than that of the primary peak, having lost some of the higher frequency components. In the time-domain trace this is manifest as the broadening of the secondary peak profile as compared with the primary peak (Fig. 2a). In the FT spectrum such reflection with absorption produces oscillations which decay at high frequencies, as seen in Fig. 2b. The algorithm therefore must be modified by applying a suitable damping function to the FT of the delta function set (Fig. 2b).

The damping function must be determined by first calculating THz absorption from the uncorrected spectrum. This is done using the standard technique which records the THz spectrum in the absence of a sample and with the sample present, and calculates absorption from this data [9]. The resulting absorption curve is then approximated by fitting a suitable polynomial. This is the damping function by which the FT of the delta function set must be multiplied. The FT of the THz signal is then divided by the modified "delta FT" as above. It may be necessary to adjust the polynomial coefficients so as to minimize oscillations in the resulting THz spectrum. The process of fitting the damping polynomial is thus performed empirically and by hand.

Note that in the presence of absorption the oscillations are reduced but not eliminated. That is because absorption alters the spectrum of the secondary peak, so that it is no longer identical to that of the primary peak. As a result, the simple representation of the time-domain data as a convolution of the primary peak and a set of delta functions is no longer correct. Applying a damping function to the FT of the delta function set allows to approximate the effect of absorption, but not to simulate it accurately. Clearly, this deviation from the approximation to a convolution becomes more significant with increased absorption. The algorithm is therefore unsuited to samples having strong absorption.

An even greater problem arises if the sample is dispersive, since in that case the distortion of the secondary peak cannot be simply modeled by modifications to the FT of the delta function set. In consequence, the algorithm cannot address strongly dispersive samples. This limitation, however, is less serious than the previous one (i.e., the requirement for low absorption), since few materials exhibit strong dispersion at THz frequencies [9,10].

3. Results

We illustrate the use of the algorithm by applying it to the data obtained from two samples: (i) a high-resistivity Si wafer and (ii) a high-density Al_2O_3 plate.

The measurements were carried out on a THz time-domain spectroscopy system of a conventional configuration, shown in Fig. 3, and described in detail elsewhere [9]. The setup employed a 60 fs Ti-sapphire laser (Spectra-Physics Tsunami). The average power of the laser was 0.9 W, of which approximately 0.8 W was used for terahertz generation from a biased GaAs emitter. Electro-optic (EO) detection with balanced photodiodes was employed to observe the THz signal. The EO detector was a ZnTe crystal cut so that the beam propagation was along its ⟨110⟩ axis. The dynamic range of the THz spectroscopy system was around 2000 in amplitude, and the usable bandwidth was from 100 GHz to 3 THz. The optical configuration was designed to provide a focused THz beam for imaging and a parallel beam for spectroscopy.

A Si wafer (460 μm thick) was chosen as an example of material that has negligible absorption at THz frequencies. The refractive index of Si is 3.4, which results in a 30% power reflection at a Si–air interface. The amplitude of the secondary reflection peak is therefore approximately 25% that of the primary peak. Fig. 4a shows the time-

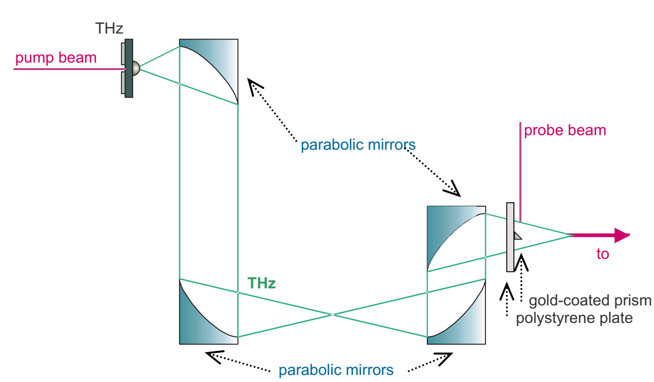

Fig. 3. A schematic drawing of the THz time-domain spectroscopy (TDS) system.

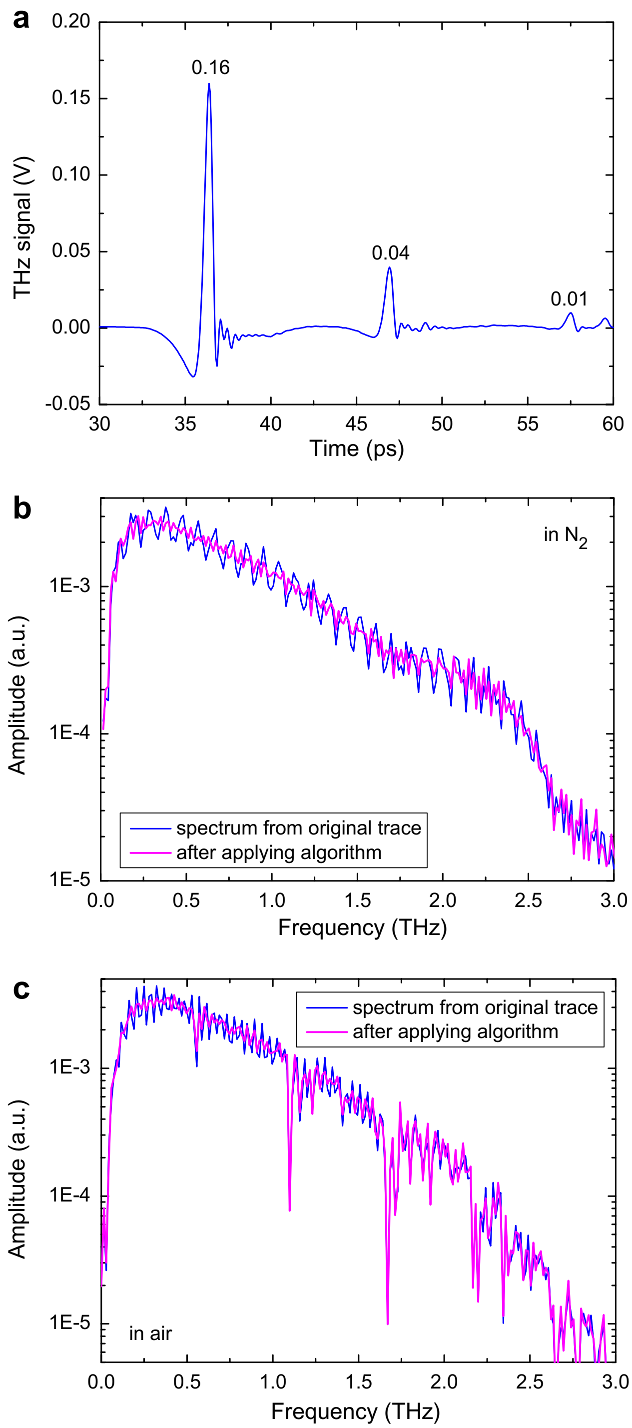

Fig. 4. Si wafer (460 μm thick): (a) the time-domain trace showing secondary peaks. Applying the algorithm to THz data obtained in (b) dry N_2, and (c) ambient atmosphere (showing water absorption lines).

domain data, while Fig. 4b demonstrates the application of the algorithm. Fig. 4c does the same in a case where the measurement was carried out in ambient atmosphere, and therefore water vapour absorption lines are evident. It is seen that the application of the algorithm does not affect peaks in the spectrum.

An Al_2O_3 plate (1 mm thick) was selected as an example of material which has significant THz absorption. The refractive index of Al_2O_3 is 3, producing a 25% power reflection at an alumina–air interface. Owing to the absorption which increases with frequency, a damping function must be employed in this case, as explained above (Fig. 2). Fig. 5 plots the calculated THz spectra before and after the application of the algorithm. As discussed above, in the case where absorption is present, the etalon oscillations are significantly reduced but not eliminated, owing to the difference in the spectral content of the primary and secondary peaks, which is difficult to model using a simple damping function.

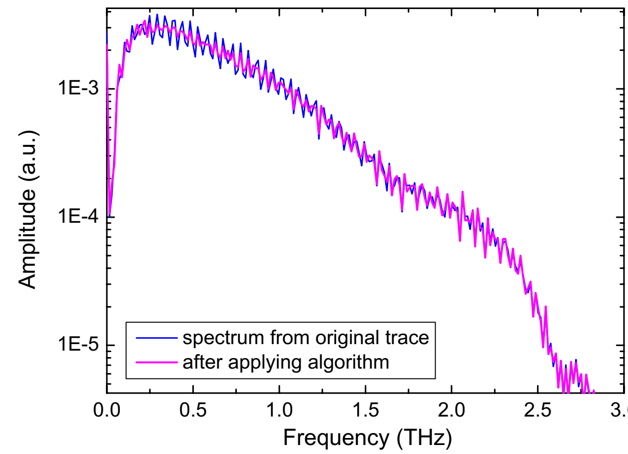

Fig. 5. Applying the algorithm to THz data from a Al_2O_3 plate (1 mm thick).

4. Conclusions

We have shown a simple algorithm for the reduction of spurious oscillations in THz spectra arising from the etalon effect in optical elements or samples. The application of the algorithm was demonstrated on data from a silicon wafer and an alumina plate. It was shown that the algorithm leaves unaffected sharp peaks in the spectrum.

The algorithm has two limitations: the samples must have low absorption and dispersion; and must be sufficiently thick that the secondary peak does not overlap with the primary peak.

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