Improved Algorithm for Material Characterization by Terahertz Reflection Imaging

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***Abstract*— We propose a new algorithm to improve the accuracy of sample characterization when the sample is measured on the imaging window of a terahertz reflection imaging system. Most existing approaches assume that the imaging window is homogenous, but we have noticed that there are small variations in thickness across such windows and that these can significantly affect the accuracy of standard approaches to extract the sample properties, particularly the absorption coefficient. Our algorithm accounts for both thickness variation across the imaging window as well as fluctuations in the incident pulse and mechanical jitter. Furthermore, our algorithm removes the need to measure the reference at every point that the sample is measured and thus reduces the imaging time.**

I. Introduction

Many terahertz applications require accurate characterization of material properties. For example, in terahertz studies of protein dynamics and hydration shell formation, the concentration dependent change in optical parameters need to be probed accurately [1, 2]. On a more macroscopic scale, the difference in optical parameters between tissues provides the contrast for tissue type characterization [3]. Experiments which require high accuracy are mostly performed using a transmission geometry system; however reflection geometry would potentially be more convenient for many investigations, such as in-vivo experiments. In reflection geometry, the extraction of parameters is very sensitive to the phase alignment between the sample and reference signal: minor misalignment will induce large errors in the characterization results. The main causes of phase misalignments include: the incident pulse fluctuation in fiber based terahertz systems, mechanical jittering of optical stages and the inhomogeneity of the imaging window.

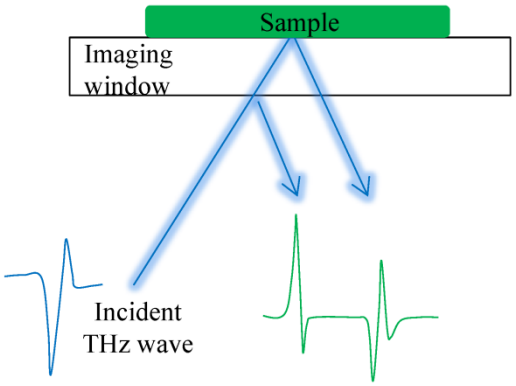

Fig. 1. The structure for sample imaging in a typical terahertz reflection system

Fig. 1 illustrates a typical terahertz reflection system that has an imaging window upon which the samples are placed for imaging. Variations in the window thickness will induce phase misalignment if the reference is taken using a single point or an area near to the sample (we will refer to this as the single reference method). Although this error could be partially removed by measuring the reference at each spatial point where the sample is measured (we will refer to this as the normal method), it is time consuming and given the fluctuations due to fibre drift and mechanical jitter, it will not be a complete solution.

The phase misalignment induced errors described above can be removed by improving the data processing algorithm. In this paper, we present the theory and equations of our improved algorithm which makes use of the reflected THz signals from both the bottom and the top of the imaging window, followed by the improvement results.

II. Theory and Equations

Our current algorithm requires three measurements for material characterization: an air measurement to use as the reference, a water measurement to calibrate the system [4], and the sample measurement.

As shown in Fig. 1, the incident terahertz pulse will result in two reflections: one from the bottom of the imaging window and the other from the top. When measuring the air (nothing is placed on the imaging window), the relationship between these two reflections which we denote as S can be expressed with Equation (1), where E_{1air} and E_{2air} represent the reflections from the bottom and top surfaces of the imaging window respectively. c is the speed of light, t denotes the transmission ratio of the electrical field, ω is the angular frequency, d_{window} is the thickness of the imaging window, and θ_i is the incident angle of the terahertz pulse. x_i and y_i are the spatial coordinates.

$$S(x_i, y_i, \omega) = \frac{E_{2air}(\omega)}{E_{1air}(\omega)} = \frac{r_{window}^{air}}{r_{air}^{window}} = f[\tilde{n}_{air}(\omega), \tilde{n}_{window}(\omega), d_{window}(x_i, y_i)] \quad (1)$$

We call this relationship the transfer function from window to air. As long as the incident angle stays the same, the transfer function will only be dependent on the refractive index of the air, the refractive index of the imaging window, and thickness of the imaging window.

The second reflection of the water measurement and the air measurement also has a relationship which we denote as Q, namely the reflection quotient between water and air. It is expressed as:

$$Q(\omega) = \frac{E_{2water}(\omega)}{E_{2air}(\omega)} = \frac{r_{window}^{water}}{r_{window}^{air}} = f[\tilde{n}_{window}(\omega), \tilde{n}_{air}(\omega), \tilde{n}_{water}(\omega)] \quad (2)$$

where r represents the reflection ratio of the electrical field and $\tilde{n}$ is the complex refractive index. From Equation (2), we can see that Q is also not affected by the incident pulse, and is a function of the complex refractive index of the window, water and air. This relationship will not change as long as the experiment environment is stable..

In our proposed algorithm, S at every spatial point on the imaging window is calculated and saved. S and Q can be used to recover the air and water signal in all of our future measurements as shown by the schematic in Fig. 2 with Equation (3) and (4). The calculated sample and air signal after baseline subtraction can be further used to calculate the optical properties of the sample.

$$E_{2air}^{calc}(x_i, y_i, t) = ifft\{S(x_i, y_i, \omega) \cdot FFT[E_{1sample}^{meas}(x_i, y_i, t)]\} \quad (3)$$

$$E_{2water}^{calc}(x_i, y_i, t) = ifft\{Q(\omega) \cdot FFT[E_{2air}^{calc}(x_i, y_i, t)]\} \quad (4)$$

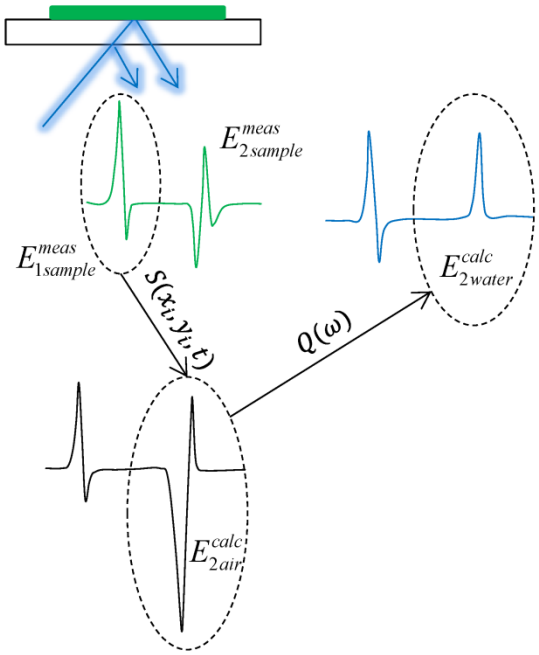

Fig. 2. This schematic shows the process to calculate the air and water signals with the transfer function S and the reflection quotient Q. The calculated signals can be used further to calculate the baseline.

S and Q are not influenced by the incident pulse which suffers from the instability caused by fibre drifts and mechanical jitters, therefore the errors in the results will be eliminated. Furthermore, since S is calculated corresponding to every spatial point on the imaging window, the phase misalignment problem due to inhomogeneity of the window thickness can also be removed.

III. Experiment Setup

Our system is a commercial terahertz time domain spectroscopy (THz-TDS) system from Menlo Systems. The system was used in 30 degree reflection mode. A circular rubber was placed on the quartz imaging window which makes it a liquid holder. Isopropanol was poured into the circular holder until the reflection from the upper surface of the isopropanol was beyond our measuring time window. The size of the THz image was 40 mm×40 mm with a resolution of 0.5 mm. Air and water were also imaged using the same parameters to calculate the transfer function and reflection quotient.

IV. Results

Fig. 3 shows the results of measuring isopropanol on top of the imaging window in a circular rubber holder. We plot the absorption coefficient at 0.45 THz across the imaging window using a linear colour scheme to highlight the variation in the result for the different algorithms. The frequency of 0.45 THz was used as it is the peak of our THz source spectrum. The different data processing methods mostly affect the result of the absorption coefficient rather than the refractive index. We see variations in the sample properties despite the sample being homogeneous. For each data processing method, the pattern of the variations is different. With the single reference method (Fig. 3.a), the absorption is smaller on the top left corner and gradually increases to the bottom right showing that the result is sensitive to the inhomogeneity of the imaging window. The "normal" method (Fig. 3.b) removes this error due to the imaging window but is sensitive to the fluctuation of the incident pulse, therefore the variation is random. In contrast with these two methods, our proposed algorithm (Fig. 3.c) can simultaneously remove both the systematic errors caused by the imaging window and those arising from the pulse fluctuation resulting in a much smaller standard deviation in the absorption coefficient, as indicated by the uniform colour in Fig. 2.c.

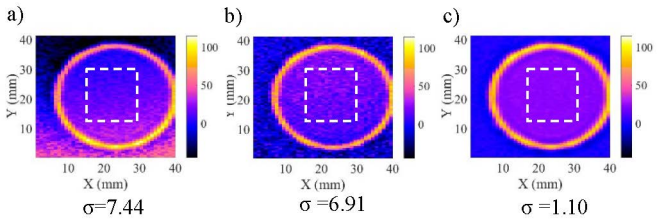

Fig. 3. Figure (a) to (c) plot the absorption coefficient at 0.45THz calculated with different methods: (a) single reference method, (b) normal method, (c) our proposed algorithm. The standard deviations (σ) of the absorption coefficient at 0.45 THz calculated using the data in the white dashed box are shown under each figure.

V. Summary

Phase misalignment is a major problem affecting the accuracy of material characterization with terahertz reflection imaging system. Fibre drift in fibre based terahertz systems, mechanical jitters, and the inhomogeneous thickness of the imaging window all contribute to the phase misalignment between the sample and the reference signals. In this paper, we propose an improved algorithm using the transfer function and reflection quotient to calculate the sample and reference signals. We validate our method by imaging the isopropanol and compare our results with the normal method and the single reference method. The spatial variation in the calculated absorption coefficient is significantly reduced. Both the error caused by incident pulse fluctuation and that due to the imaging window are efficiently eliminated. Further validation of our

proposed algorithm on its stability and accuracy is described in our recent work [5].

VI. Acknowledgements

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