

Improved sample characterization in terahertz reflection imaging and spectroscopy

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Abstract: For imaging applications involving biological subjects, the strong attenuation of terahertz radiation by water means that terahertz pulsed imaging is most likely to be successfully implemented in a reflection geometry. Many terahertz reflection geometry systems have a window onto which the sample is placed – this window may introduce unwanted reflections which interfere with the reflection of interest from the sample. In this paper we derive a new approach to account for the effects of these reflections and illustrate its success with improved calculations of sample optical properties.

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OCIS codes: (300.6495) Spectroscopy, terahertz; (120.4825) Optical time domain reflectometry; (080.2740) Geometric optical design; (110.6795) Terahertz imaging

References and links

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1. Introduction

Terahertz pulsed imaging is a non-destructive, non-ionising imaging modality. Terahertz pulsed imaging is still in its infancy with many groups worldwide investigating potential applications in non-destructive testing, chemical analysis, security screening and medical imaging [1-5]. Terahertz radiation probes intermolecular vibrations such as hydrogen bonds which occur naturally in biological systems [6, 7]. Additionally, terahertz imaging methods, using sub picosecond pulses of radiation are able to obtain an axial resolution of around 40 microns (in air but this is dependent on the refractive index of the sample and the bandwidth of the system [8]). Thus, terahertz imaging and spectroscopy could potentially be used to probe both the structure and composition of biological samples by measuring directly their absorption and refractive index.

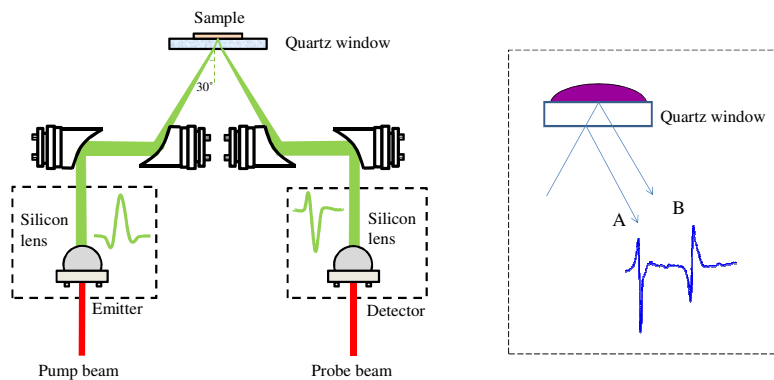


Fig. 1. Schematic diagram to illustrate how the terahertz beam is focused on to the quartz window and sample. The resulting reflections of the incident terahertz light are depicted in the large dashed box.

Terahertz radiation is strongly attenuated by water which is often a large fractional component of biological samples; therefore, for measurements to be performed in transmission geometry the sample must be very thin (typically less than 500 microns). This is only possible for samples that lend themselves to be cut into very thin slices, for example, excised soft tissues. Wallace et al. measured the frequency dependent refractive index and absorption of excised basal cell carcinoma samples [9]. However, there have been very few reports on the terahertz properties of such samples. If terahertz imaging is to be used in the future for medical applications, it is likely to be more feasible if conducted in reflection

geometry, a more practical implementation from which accurate measurements of the tissues properties can also be extracted [10-12]. In this geometry, samples are typically placed on a sample window. The window is made of a material with minimal absorption at terahertz frequencies such as silicon or z-cut quartz. To date, it has been difficult to extract accurate absorption data in reflection geometry as it is contained within the phase information of the measurement [13] which is sensitive to system artifacts.

The pulsed terahertz radiation is focused onto the top surface of the sample window, as illustrated in Fig. 1, such that the main pulse i.e. the sample reflection (B) due to the window/sample interface can be measured. However, there is also a reflection (A) from the lower surface of the window. The main part of this pulse is often ignored in time-gated detection systems but it has an enduring signal or “ringing” which interferes with the sample reflection (B).

Previous work by Jepsen et al. has shown how terahertz reflection spectroscopy could be used to characterise alcohol solutions inside bottles [14]. In their work, they use Fresnel equations to simulate expected sample reflections from the inside of the bottle. They report that the experiment reproduces the simulation quite well and that the experimental details left out of the simulation do not significantly influence the result [14]. In this paper, we exploit the difference between simulated and measured reflections to determine a baseline offset to correct for errors due to the “ringing”. This baseline is then used to improve calculations of the complex refractive index in reflection.

Methods to remove the effects of the ringing previously reported have taken a baseline measurement of the sample window with an identical window placed on top [15], as illustrated for a quartz window in Fig. 2(b).

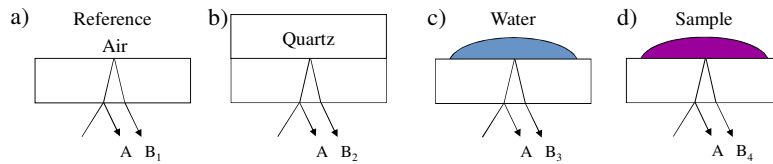


Fig. 2. Schematic diagrams to illustrate the measurement configurations for reference (a), baseline (b), water (c) and sample (d) data acquisition.

Since the windows are identical, there should be no reflection from the interface between the sample window and the second window. The resulting reflection should only represent the effects of the ringing and should be continuous and extend into the region over which to measure reflection A. We refer to this as the “baseline” measurement. However, in practice it is very difficult to achieve perfect contact between the two windows and consequently the measured signal in configuration Fig. 2(b) is not only due to the ringing from reflection A but also contains a small reflection (B_2) due to the slight air gap between the windows (which causes a refractive index mismatch). Another possible approach would be to apply a thin layer of index matched liquid to the original window so as to prevent air gaps forming between the two windows when taking a baseline measurement. However, in practice it is not possible to perfectly match both the refractive index and absorption coefficient and so this method would still introduce some unwanted reflections.

Some reflection systems use a thicker window of higher refractive index (such as silicon) to provide a greater optical delay between the reflections on the lower and upper surfaces [16]. Additionally since the ringing has further to propagate before it interferes with the sample measurement, it is likely to be weaker. However, it would still be of significance for accurate sample characterization. In the system used here there is a requirement for the window to be optically transparent to allow for image registration and thus quartz is used. However, using a thicker quartz window could cause unwanted dispersion. In order to determine the sample properties accurately through reflection spectroscopy and imaging, we

need to be able to measure the baseline more precisely and reliably. In this paper we derive a new approach to achieve this goal. This method can be easily implemented and can also be applied to reflection systems with different angles of incidence.

2. Theory

Our novel method is to use accurate, room temperature, terahertz pulsed transmission spectroscopy (TPS) data of a standard material such as water to simulate the reflected terahertz pulse for a given input pulse. We have previously used double Debye theory in our finite difference time domain simulations of water [17]. In this paper we use the measured frequency dependent optical properties of water in conjunction with a measured reference pulse and Fresnel equations to predict the reflection off water. We chose water for this as it will naturally make perfect contact with the quartz window. By comparing the simulated water reflection with the measured water reflection, the effect of the ringing can be determined and this ringing can then be accounted for in calculations of unknown samples such that the optical properties of these samples can be determined more accurately. This process is summarized schematically in Fig. 3.

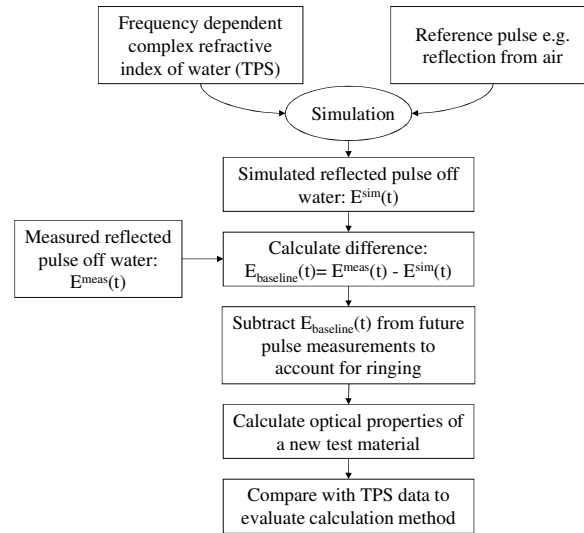


Fig. 3. Flow chart to summarize the new baseline approach.

The measured electric fields of the pulses reflected off the quartz/air and quartz/water interfaces (corresponding to the reflections B_1 and B_3 in Fig. 2) in the time domain are notated by $E_{air}^{meas}(t)$ and $E_{water}^{meas}(t)$ respectively. The measured electric field is the superposition of the actual reflection due to the interface with the baseline reflection, $E_{baseline}(t)$, due to the ringing:

$$E_{air}^{meas}(t) = E_{air}(t) + E_{baseline}(t) \quad (1)$$

$$E_{water}^{meas}(t) = E_{water}(t) + E_{baseline}(t) \quad (2)$$

Where $E_{water}(t)$ and $E_{air}(t)$ are the actual reflections in the time domain at the quartz/water and quartz/air interfaces respectively. The reflected time domain pulses are Fourier transformed to obtain the corresponding frequency domain spectra, in this case $E_{water}(\omega)$ and $E_{air}(\omega)$.

For the actual reflected pulses, assuming they are s-polarized, the following Fresnel theory can be used to determine their ratio in the frequency domain, M , in terms of the optical properties of the quartz, water and air:

$$M = \frac{E_{\text{water}}(\omega)}{E_{\text{air}}(\omega)} = \frac{(\tilde{k}_{\text{quartz}} \cos \theta_{\text{quartz}} - \tilde{k}_{\text{water}} \cos \theta_{\text{water}})(\tilde{k}_{\text{quartz}} \cos \theta_{\text{quartz}} + \tilde{k}_{\text{air}} \cos \theta_{\text{air}})}{(\tilde{k}_{\text{quartz}} \cos \theta_{\text{quartz}} + \tilde{k}_{\text{water}} \cos \theta_{\text{water}})(\tilde{k}_{\text{quartz}} \cos \theta_{\text{quartz}} - \tilde{k}_{\text{air}} \cos \theta_{\text{air}})} \quad (3)$$

Where, $\tilde{k} = \frac{\omega}{c}n(\omega) - \frac{i}{2}\alpha(\omega)$ is the frequency dependent complex refractive index of a medium with refractive index n and absorption coefficient α . The angle of incidence of the light entering the quartz is θ_{quartz} , and the angles of refraction in air and water are θ_{air} and θ_{water} respectively. Values for \tilde{k}_{air} and θ_{air} are known. Spectroscopy data acquired in transmission geometry are used for calculating $\tilde{k}_{\text{quartz}}$ and \tilde{k}_{water} . The angles θ_{quartz} and θ_{water} can be calculated from Snell's law: $n_{\text{quartz}} \sin \theta_{\text{quartz}} = n_{\text{air}} \sin \theta_{\text{air}} = n_{\text{water}} \sin \theta_{\text{water}}$.

From the above three equations, we obtain the following formula for $E_{\text{baseline}}(\omega)$:

$$E_{\text{baseline}}(\omega) = \frac{E_{\text{water}}^{\text{meas}}(\omega) - M \cdot E_{\text{air}}^{\text{meas}}(\omega)}{1 - M} \quad (4)$$

Where $E_{\text{water}}^{\text{meas}}(\omega)$ and $E_{\text{air}}^{\text{meas}}(\omega)$ are the Fourier transforms of $E_{\text{water}}^{\text{meas}}(t)$ and $E_{\text{air}}^{\text{meas}}(t)$ respectively. The simulated $E_{\text{baseline}}(t)$ can then be calculated by taking the inverse Fourier transforms of $E_{\text{baseline}}(\omega)$ in Eq. (4). This simulated baseline is then used to calculate the actual reflected pulse:

$$E(t) = E^{\text{meas}}(t) - E_{\text{baseline}}(t) \quad (5)$$

The actual electric field is then used to obtain the complex refractive index of a test material following Fresnel theory as detailed in reference [11].

3. Results and discussion

To test our theory, we performed room temperature measurements of air, quartz, distilled water and isopropanol using our reflection terahertz imaging system (TPI Imaga1000, TeraView Ltd, UK). The system has been described in detail in our earlier papers [11, 18]. The liquid samples were placed on the quartz window to form a depth of at least 1 mm to ensure the reflection off the liquid/air interface was excluded from the detected signal.

For each measurement, a small area of the sample was raster scanned and a grid of pixels (25 by 25) was collected. These measurements were repeated four times and the mean values are used for this study.

3.1 Calculated baseline

Using the measurements of water and air, we calculated the simulated baseline using the theory above. The result is plotted in Fig. 4 along with the measured baseline using the extra quartz window (as illustrated in Fig. 2(b)). From the time domain waveforms, it can be seen that the intensities of both these two baselines are of the same order. However, considerable difference lies in their main pulses (from 15 to 25 ps).

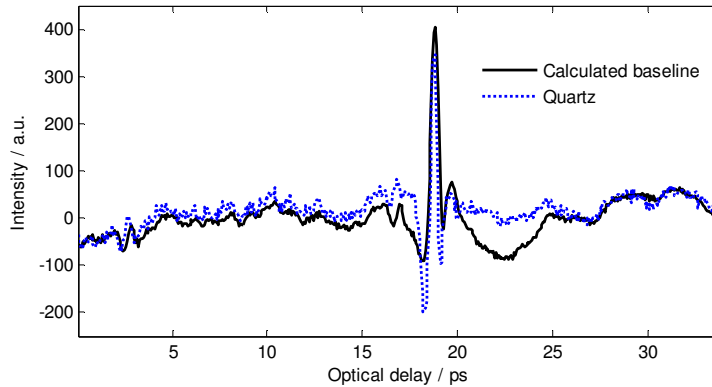


Fig. 4. Time domain waveforms of the calculated baseline and the measured baseline.

3.2 Baseline validation

We have calculated the optical properties of our test material, isopropanol, using the new simulated baseline and compared them in Fig. 5 to those obtained by the old baseline method (measured with the extra quartz window in place). Additionally, we have transmission spectroscopy data of the isopropanol which can be considered to be the most accurate data for the sample.

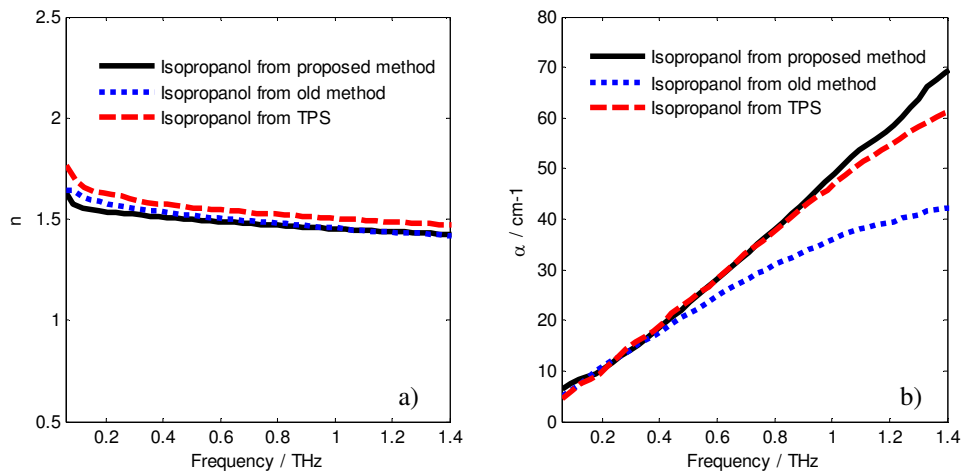


Fig 5 The refractive index (a) and absorption coefficient (b) of isopropanol using our proposed baseline method and the old baseline method compared to those from TPS measurements.

As we can see from Fig. 5(b), the absorption coefficient calculated using the new baseline method matches the TPS data much more closely than when the old baseline was used in the calculation. This is most likely to be because when calculating the optical properties in a reflection geometry, the absorption coefficient is predominantly dependent on the phase information and this is very sensitive to the experimental setup and protocol. Since the water makes perfect contact with the quartz sample window, our method using the water data to determine the baseline has more accurate phase information than the baseline from placing a quartz window on top of the sample window and thus the absorption coefficient calculation is much improved and the frequency range of agreement with the TPS data is approximately doubled from upto 0.5 THz to upto 1 THz. This is also relevant to biomedical applications as

the most interesting frequency range for tissue measurements has been shown to be up to 1 THz [9]. The improvement is not so pronounced for the refractive index data. In reflection geometry the refractive index is predominantly dependent on the amplitude rather than the phase and so is well determined in both our calculations. Conversely, the TPS refractive index is predominantly dependent on the phase information and so is potentially less reliable than the refractive index calculated in reflection geometry. However to compensate for this, the TPS data is acquired over a longer time delay with multiple averaging and so only a slight discrepancy is seen between the TPS data for both refractive index calculations. Therefore with this improved baseline calculation both the absorption coefficient and refractive index can be well determined in reflection geometry over a greater frequency range.

For terahertz pulsed imaging, the impulse function in the time domain is important for signal processing as well as terahertz image reconstruction. It is typically deconvolved from the measured sample and reference signals [19, 20]. The impulse response of a sample can also be improved by this new baseline method as in Eq. (6), where a Gaussian filter is applied to remove both the low and high frequency noise components.

$$FFT(\text{Impulse function}) = FFT(\text{filter}) \times \frac{FFT(E_{\text{sample}}^{\text{meas}}(t) - E_{\text{baseline}}(t))}{FFT(E_{\text{air}}^{\text{meas}}(t) - E_{\text{baseline}}(t))} \quad (6)$$

4. Conclusion

In conclusion, we have demonstrated a new method to account for the ringing artifacts observed in terahertz pulsed reflection imaging due to the lower surface of the sample window required in the majority reflection imaging and spectroscopy systems. This method has a straightforward protocol which enables the reference measurements to be taken reliably and easily such that the effects of the ringing and subsequently other system artifacts can be determined and accounted for in calculations. In this way we can improve calculations of the complex refractive index of samples measured in a reflection geometry.

Acknowledgments

This work was partially funded by the Research Grants Council of the Hong Kong Government and the Shun Hing Institute of Advanced Engineering, Hong Kong.