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Terahertz Optical Constants of Air by Characteristic Matrix Method

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ABSTRACT*: In this paper, terahertz optical constants of 12 % RH air are reported by using characteristic matrix method. In the terahertz time-domain spectroscopy experiment, the radiation was generated by optical rectification and detected by electro-optic sampling in ZnTe. The transmission of radiation through the five layered reference system nitrogen gas-teflon-nitrogen gas-quartz-nitrogen gas and sample system air-teflon-air-quartz was modeled by characteristic matrix (CM) method. An error function involving the experimental transmission coefficient and transmission coefficient modeled by the CM method was minimized to extract the optical constants of air at 12% RH.*

KEYWORDS-*Terahertz, far infrared, Optical constants, Characteristic matrix method, multilayer*

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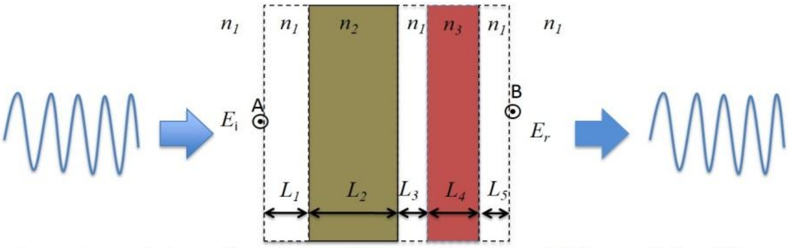
I. INTRODUCTION

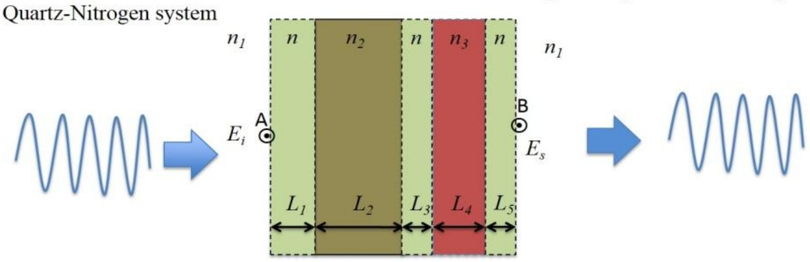
Terahertz time-domain spectroscopy (THz-TDS) [1] is an efficient technique to characterizeplanar samples of known [2–4] or unknown thickness [4–7]. In the transmitted THz waveform through a layered system like the ice films deposited on a planar substrate attached to the cold finger of a cryostat with planar pass through windows, we see echoes due to reflections from interfaces of various media: windows of the cryostat, the sample understudy that was grown on a planar substrate, and the substrate. For the extraction of optical constants, one usually truncate the THz waveform well before the first echo and computes the Fourier transformations of the reference and sample waveforms[8]. The transmission coefficient defined as the ratio of sample spectrum to the reference can show absorption lines in the sample but the full width at half maxima (FWHM) of the absorption features will be limited by the experimental spectral resolution which is the inverse of length of the THz waveforms. For the better frequency resolution, we need longer time-domain THz waveforms. But in the longer THz waveforms we have echoes due to the sources mentioned earlier that make the sample and reference spectra possess interference fringes. Here, we report on a method in which we made use of characteristic matrix(CM) method [9] to analyze longer waveforms with echoes due to each layer of a layered material like air-telfon-air-quartz-air. Recently, a similar kind of analysis was used for a two dimensional electron gas sample in magnetic fields [10]. With this method, this paper shows the analysis of air spectrum with 5 GHz resolution. Though a spectral resolution of 7 GHz was demonstrated with the waveguide THz-TDS [11], it is not implemented here because it is not ideal for studying layered samples prepared in situ like in a cryostat by vapor deposition. Water vapor has been studied by many groups extensively [12-23]. The pure rotational transitions of water vapor occur in terahertz frequency range [12]. The terahertz absorption by water vapor was observed in grating based spectrometers [12] and Fourier transform infrared spectroscopy [12–15], and tunable far infrared spectroscopy [20]. The pure rotational spectrum of water vapor was also studied by terahertz time domain spectroscopy [16–19, 23]. Specific line broadening due to the presence of atmospheric gases at low pressures was studied recently by several groups [24–27]. The water vapor was chosen to test the CM method based analysis because of the plenty of literature available to compare the results.

II. Experimental

A standard THz time-domain spectrometer was used for the experiment, in which THz radiation was generated by optical rectification inside a ZnTe crystal of 1mm thick and (110) orientation. The THz radiation is detected by electro-optic sampling method inside a 1mm thick (110) oriented ZnTe chip cemented on a 2 mm thick (100) ZnTe. A teflon block was placed at a distance of 24 mm from the generating ZnTe, a quartz block is placed at a distance of 489 mm from the teflon block, and the distance between the quartz substrate and the detector ZnTe crystal is 464 mm. The entire experiment is purged with dry nitrogen gas to maintain a relative humidity less than 1% for the reference scan and for the sample scan the humidity was maintained at 12% RH. Both the sample scan and reference scan are acquired for 200 ps long duration.



a. A wave transmission as the reference THz waveform through Nitrogen-Teflon-Nitrogen-Quartz-Nitrogen system



b. A wave transmission as the sample THz waveform through Air-Teflon-Air-Quartz-Air system

Figure1: (a) The wave propagation through the reference system. (b) The wave propagation through the sample system.

III. Theory

Figure 1 shows the systems for reference scan and sample scan. The characteristic matrix for the reference system can be written as

$$M=\begin{bmatrix}\cos\beta_1 & \frac{-i}{q_1}\sin\beta_1\\ \frac{-i}{q_1}\sin\beta_1 & \cos\beta_1\end{bmatrix}\begin{bmatrix}\cos\beta_2 & \frac{-i}{q_2}\sin\beta_2\\ \frac{-i}{q_2}\sin\beta_2 & \cos\beta_2\end{bmatrix}\begin{bmatrix}\cos\beta_3 & \frac{-i}{q_3}\sin\beta_3\\ \frac{-i}{q_3}\sin\beta_3 & \cos\beta_3\end{bmatrix}\begin{bmatrix}\cos\beta_4 & \frac{-i}{q_4}\sin\beta_4\\ \frac{-i}{q_4}\sin\beta_4 & \cos\beta_4\end{bmatrix}\begin{bmatrix}\cos\beta_5 & \frac{-i}{q_5}\sin\beta_5\\ \frac{-i}{q_5}\sin\beta_5 & \cos\beta_5\end{bmatrix}$$

Here, $\beta_i=\frac{2\pi n_i L_i}{c}$, $q_i=\frac{1}{n_i}$ for i=1, 2, 3, 4, 5. Also, $n_1=n_1$, $n_2=n_2$, $n_3=n_1$, $n_4=n_3$, and $n_5=n_1$. The ratio of the amplitudes of the transmitted electric field at B and the incident electric field at A is given by $t_r=\frac{2q_1}{(M_{11}+M_{12}q_1)q_1+(M_{21}+M_{22}q_1)}$. Here, M_{ij} is the i^{th} row and j^{th} column element of the matrix M.

The characteristic matrix for the sample system can be written as

$$N=\begin{bmatrix}\cos\beta_6 & \frac{-i}{q_6}\sin\beta_6\\ \frac{-i}{q_6}\sin\beta_6 & \cos\beta_6\end{bmatrix}\begin{bmatrix}\cos\beta_7 & \frac{-i}{q_7}\sin\beta_7\\ \frac{-i}{q_7}\sin\beta_7 & \cos\beta_7\end{bmatrix}\begin{bmatrix}\cos\beta_8 & \frac{-i}{q_8}\sin\beta_8\\ \frac{-i}{q_8}\sin\beta_8 & \cos\beta_8\end{bmatrix}\begin{bmatrix}\cos\beta_9 & \frac{-i}{q_9}\sin\beta_9\\ \frac{-i}{q_9}\sin\beta_9 & \cos\beta_9\end{bmatrix}\begin{bmatrix}\cos\beta_{10} & \frac{-i}{q_{10}}\sin\beta_{10}\\ \frac{-i}{q_{10}}\sin\beta_{10} & \cos\beta_{10}\end{bmatrix}$$

Here, $\beta_i=\frac{2\pi n_i L_i}{c}$, $q_i=\frac{1}{n_i}$ for i=6, 7, 8, 9, 10. Also, $n_6=n$, $n_7=n_2$, $n_8=n$, $n_9=n_3$, $n_{10}=n$ and $L_6=L_1$, $L_7=L_2$, $L_8=L_3$, $L_9=L_4$, and $L_{10}=L_5$. The ratio of the amplitudes of the transmitted electric field at B and the incident electric field at A is given by $t_s=\frac{2q_1}{(N_{11}+N_{12}q_1)q_1+(N_{21}+N_{22}q_1)}$.

The ratio of the transmitted field through the sample system and the reference system can be written as

$$T=\frac{(M_{11}+M_{12}q_1)q_1+(M_{21}+M_{22}q_1)}{(N_{11}+N_{12}q_1)q_1+(N_{21}+N_{22}q_1)}$$

We upload the reference and sample THz waveforms into our MATLAB program and compute their complex Inverse Fourier transformations. We also compute the complex transmission coefficient by taking the ratio of

Inverse Fourier transformations of sample and reference waveforms. We optimize the error function [3] shown below to extract optical constants of the air.

$$\left[\log|T|-\log|Te|\right]^2+\left[Arg(T)-Arg(Te)\right]^2 \text{--------(1)}$$

Here, *Te* is experimental transmission coefficient, *T* is characteristic matrix method based transmission coefficient, and |*T*| and *Arg(T)* stand for modulus, and argument of *T* respectively. The optimization is done by *patternsearch* function of MATLAB.

IV. Results

4.1. THz transmission through reference and samples

The THz waveforms of 200 ps long transmitted through the five layered reference and sample systems are shown in Figure 2. The probe step size of 0.05 ps and lock-in integration time of 1 sec are used for these scans. The Figure 2 shows the echoes due to the teflon block, quartz substrate and the air column 1 which is between generating ZnTe crystal and the teflon block.

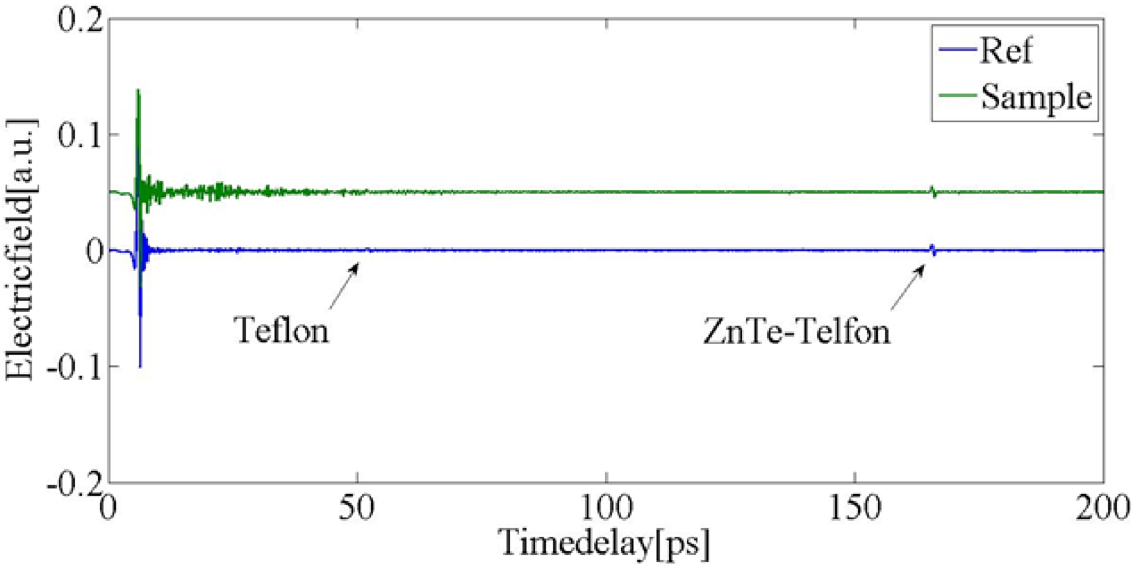


Figure2: Terahertz waveforms transmitted through the reference and sample systems

4.2. Extraction of optical constants of airThe complex inverse Fourier transformations of the waveforms are calculated to get their spectra. Since the waveforms are of 200 ps length, the spectral resolution is 5 GHz. The ratio of the sample spectrum to the reference spectrum is defined as transmission coefficient. The error function used by Duvillaret [3] involving the experimental transmission coefficient and the transmission coefficient shown in equation (2) is optimized by *patternsearch* algorithm of MATLAB for each of the frequencies between 0.2 THz and 2 THz with L_1= 24 mm, L_2= 4.82 mm, L_3= 489 mm, L_4 = 2 mm, L_5 = 464 mm. Also, n_1 = 1, n_2= 1.44+0.002i, n_4 = 2.1+i0.0024.

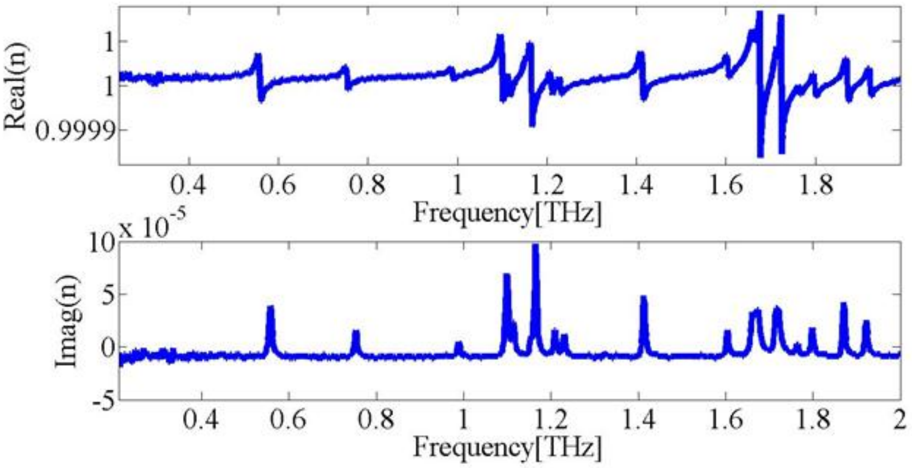


Figure 3: Real and imaginary parts of the refractive index of the air.

There were about 16 absorption lines observed for air in 0.2-2 THz. These lines were reported to be due to pure rotations of water vapor molecules [20]. The absorption center frequencies match well with those reported in ref [20]. Figure 3 shows the real and imaginary parts of the refractive index of air.

V. Conclusion

In this paper, THz optical constants of air at 12% RH in 0.2-2 THz are reported using the terahertz time-domain spectroscopy and characteristic matrix method. Both the sample and reference systems were five layered systems.

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