Complex Permittivity of Pure Water Measured by Vector Network Analysis at W-Band

Bin Yang*, Kastriot Shala, Xiaoming Liu, Hansheng Su and Robert S. Donnan*
School of Electronic Engineering and Computer Science, Queen Mary University of London, Mile End Road, London, E1 4NS, UK.
E-mail*: bin.yang@elec.qmul.ac.uk; robert.donnan@elec.qmul.ac.uk

Abstract. Preliminary pure-water transmittance measurements over the W-band (75 – 110 GHz) are performed using a well-designed quasi-optical bench and vector network analyser (VNA/QO). The measurements are an initial trial to explore vector network analysis in studies of micro-biological systems.

1. Introduction
Water, the commonest and most studied liquid on earth, continues to warrant detailed metrology in view of its varied complex influences in the function of micro-biological systems – e.g. proteins. Terahertz (THz) spectrometric investigations of condensed-phase biological systems are relatively new [1, 2 and 3] and research interests cover: simple crystalline forms of amino acids; carbohydrates and polypeptides to the more complex aqueous forms of small proteins; DNA and RNA. However, the role of water in bio-molecular dynamics is still unclear and so careful acquisition of reference data from pure water is warranted. In this paper therefore, preliminary pure-water transmittance measurements over the W-band (75 – 110 GHz) are performed using a vector network analyser and quasi-optical bench (VNA+QO).

2. Measurement System
A well-designed, quasi-optical transmissometer [4] driven by a HP N5244A Vector Network Analyzer (VNA) from 75 to 110 GHz has been used for this work. Compared with FTIR and THz-TDS, the Agilent VNA (spanning DC to 1 THz), is able to offer a greater dynamic range and signal-to-noise ratio of around 100 to 140 dB. The VNA also provides greater spectral resolution down to 1 MHz. This is superior to a typical 3 GHz resolution for TDS and FTIR interferometers [5]. The plane-wave angular-spectrum of a beam having a Gaussian amplitude distribution at its beam-waist of width 50mm is of Gaussian form with an angular-width near to 1 degree at 60 GHz and proportionally smaller than this for higher frequencies [6]; furthermore, the beam’s angular-width narrows appreciably as the beam refracts into the sample. This small angular-width ensures that the transmissometer essentially measures the sample-plate’s plane-wave transmittances. A large sample-plate is required (width 100 mm) in order that the beam is negligibly truncated at the edges of the
plate. It is also quite easy and simple to extend the spectrometer to THz energies by using the same quasi-optical circuit, by replacing only the corrugated feed-horns with a higher frequency band pair.

Conventional methods such as FTIR and THz-TDS have been greatly restricted to using powdered or lyophilized samples due to strong attenuation of THz frequencies by water. Our study has therefore developed a new bespoke cuvette system enabling analysis of bio-molecules and water in aqueous solution. The cuvette system consists of two 1.1 mm thick boron glass plates (a material generally transparent over millimeter and sub-millimeter wavelengths) with a 0.28 mm spacer (four metallic corner-located pads creating a constant gap between the two plates). Inlet and outlet valves are placed at opposite ends of the plates for flushing without the need to dismantle the cuvette.

3. Theoretical Debye Model for Water Analysis

The structure of a 3-layer system i.e. glass-water-glass can be represented in a corresponding 3-term product ABCD matrix. Based on the materials’ dielectric properties and thicknesses, the transmittance matrix is:

\[
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\begin{pmatrix}
A_w & B_w \\
C_w & D_w
\end{pmatrix}
\begin{pmatrix}
A_g & B_g \\
C_g & D_g
\end{pmatrix} = 2A + B + C + D.
\]

(1)

Where, subscript ‘g’ stands for boron glass and ‘w’ stands for water. The detailed equations of A, B, C and D for each layer are referenced from [7]. Therefore, the transmittance (T) and reflection (R) of the structure are

\[
T = \frac{2}{A + B + C + D}; \quad R = \frac{A + B - C - D}{A + B + C + D}.
\]

(2)

Fig.1: Temperature-dependent dielectric constant of pure water at W-band based on the Double Debye Model (suitable for frequencies below 1 THz): (left-plot) real part of the complex permittivity and (right-plot) imaginary part. The bold line is for 24.4°C, the dashed for 25°C and the light for 26.2°C.
The permittivity of boron glass is non-dispersive over the W-band at 4.463+0.066, and the transmittance loss is very low with \( \tan(\delta) \approx 10^{-3} \). In 1991, Liebe et al [8] summarised a large volume of published experimental permittivity data of liquid water, applied them, and expressed a standard dispersion formula for the permittivity of water from 0.1 to 1 THz. The model is made from two relaxation terms, and the theoretical permittivity of pure water with temperature dependence is plotted in Fig.1. From Fig.1, the permittivity variations are small but clear when the temperature is slightly changed. Clear differences are therefore expected in experimental transmittance spectra.

4. Results and Discussion

Separate pure water tests were repeated on three consecutive days, with ambient temperature varying slightly on each. In Fig.2 (left), the results from the three days are plotted together. Small differences are observed as expected. Based on the Debye model and the free-space 3-layer ABCD model, the theoretical transmittance spectra is compared with the experimental data as shown in Fig. 2(right). The observed difference could arise for two reasons: one, the theoretical permittivity, according to the Debye model holds from 100 GHz and up, but our horns are designed to operate from 75 GHz. The second may be due to mechanical effects on the water by the close-lying plates.

![Fig.2: (left) Measured glass/water/glass transmittance spectra (upper plot is the transmittance amplitudes and lower is the phase): black is at 24.4°C, blue 25°C and red 26.2°C; (right) theoretical 3-layers transmittance at 25°C based on the ABCD model (blue dotted line) compared with experimental data.](image)

The measurements are part of an initial on-going trial to explore the capabilities of vector network analysis for the study of soft condensed systems. More refined temperature- and pressure-controlled sample holders are required and such are being developed. The VNA/QO apparatus and methods is soon to be extended to higher bands of the sub-THz domain for analysis of amino acids.

5. Conclusions

The apparatus of VNA/QO and ABCD signal processing is seen in trials to-date to enable high measurement stability and repeatability from bulk pure-water tests. The aim is to apply these further in studies of biological water and other biological samples in sub-THz bands where response is expected but as yet not measured.
The errors shown in Fig.2 between experiments and model are seen to be less at the cut-on frequency of validity for the Debye model; however, further model explorations and measurement system characterisation are needed to expose systematic errors.

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