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Accurate Parameter Extraction From Liquids Measured Using On-chip Terahertz Spectroscopy

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***Abstract*—We introduce a method for estimating the permittivity of liquid samples measured using integrated microfluidic/planar Goubau line terahertz waveguides, in which simulation results are combined with practical data to enable more accurate frequency-dependent analysis.**

I. INTRODUCTION AND BACKGROUND

TERAHERTZ time-domain spectroscopy (THz-TDS) is of interest for the investigation of bio-molecular dynamics [1]. Free space THz-TDS is a well-established technique for the extraction of sample parameters such as absorption and permittivity. However, the strong absorption of many liquid samples limits the applicability of such techniques in the study of biological molecules in an aqueous environment. On-chip waveguides that support travelling waves on a surface-defined conductor offer a potential solution, allowing an evanescent field to probe proximal samples, with a significantly reduced attenuation when compared to free space systems.

On-chip picosecond current pulses can be generated and detected using Goubau line devices with integrated photoconductive semiconductors. A THz signal, generated by a photoconductive switch under pulsed laser illumination, is coupled into an overlaid planar Goubau line (PGL), used for sensing, and is then measured using lock-in detection at a second switch. A radial electric field, coupled to the guided PGL mode, is used to probe overlaid materials, and has an extent of the order of 100 µm, allowing the dielectric properties of samples placed close to the PGL to be calculated.

Previously, spectroscopy of solid polycrystalline samples has been demonstrated successfully using on-chip THz devices. However, the use of such technology is known to be problematic when measuring liquid samples, since abrupt changes in permittivity introduced by integrated microfluidic channels (required to contain the liquid-under-test, LUT) result in unwanted time-domain etalons [2]. In our previous work, these reflections were removed by locating the channel on the underside of a thin (50-µm-thick) substrate, and by increasing significantly the channel dimensions (thereby removing the interfaces from the sensing region). The LUT then covers the entirety of the PGL, increasing measurement sensitivity.

Calculating the dielectric properties of materials overlaying PGL systems using analytic methods is a non-trivial task, compared with alternative geometries such as coplanar or microstrip, owing to the lack of identifiable boundary conditions [3]. However, the relative advantages of PGLs for spectroscopic applications create a demand for numerical approximations that allow calculation of sample properties.

The extraction of dielectric sample properties from PGL measurements has been based previously on the assumption that the probing THz-frequency evanescent field is distributed symmetrically about the transmission line under all operating conditions. Here, we show that the field extent (both into and out of the substrate) is strongly dependent on the properties of the LUT, and that this assumption does not therefore allow accurate parameter estimation. In this work, liquid samples were measured using a PGL with an overlaid fluidic channel, all fabricated on a quartz substrate. Frequency-domain simulations of the device response to an LUT were performed with HFSS (Ansys, Inc.) between 0.1 THz and 1 THz, in which the LUT permittivity ε_{lut} was varied from $\varepsilon_{\text{lut}} = 1$ to $\varepsilon_{\text{lut}} = 6$, in increments of 0.25.

As shown in Fig. 1(a), the extent of the electric field about the PGL (and therefore the interaction between the field and the sample) is reduced at higher frequencies. The symmetry of the field distribution about the PGL is dependent on the ratio between the substrate and superstrate permittivities [4]. Given a quartz substrate ($\varepsilon \sim 3.8$), the results in Fig. 1(a) show how the field is more evenly distributed for a sample where $\varepsilon_{\text{lut}} = 3$ than for an air sample ($\varepsilon_{\text{lut}} = 1$). These simulations show that a numerical model incorporating both the frequency and permittivity-dependent field distributions is required to calculate a better approximation of the sample parameters.

II. RESULTS

A 1-mm-long PGL was patterned on a 100-µm-thick quartz substrate, over which a 6-µm-thick insulation layer of benzocyclobutene (BCB) was applied. The insulation layer acts as a barrier between the LUT and the transmission line. BCB was selected as it is highly impermeable, and is sufficiently thermally stable that it is not damaged by the focused lasers used to generate and detect the THz fields. A 100-µm-deep polydimethylsiloxane (PDMS) channel was irreversibly bonded to the BCB-coated substrate using an amine–epoxy bonding technique [5]. Inlet and outlet ports were formed with silicone tubing, and the inlet was connected to a syringe pump to provide control over the flow of the LUT. Measurements

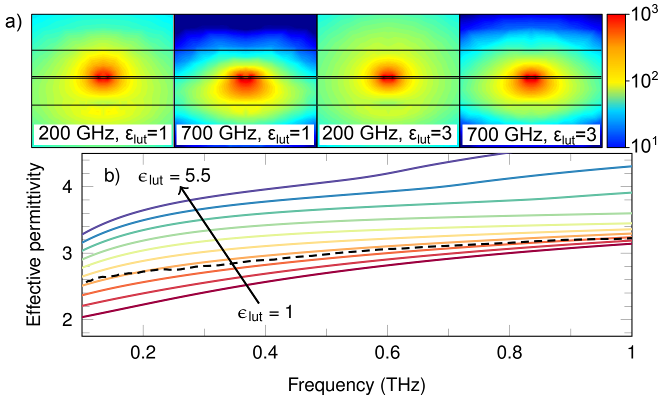

Fig. 1. (a) The simulated cross-sectional field distribution (400 µm × 400 µm crop shown) about a PGL formed on a 100-µm-thick quartz substrate at 200 GHz and 700 GHz, with a sample of varying permittivity above the substrate. (b) The effective permittivity of a simulated device for a range of sample permittivities in increments of 0.5 (solid), and the experimentally measured effective permittivity of a device filled with propan-2-ol (dashed).

were made by recording spectra of an air-filled reference channel, and an LUT. Between each measurement, the previous sample was removed and the channel was cleaned by flushing with propan-2-ol, and purging with dry air (<1 % humidity).

The effective permittivity of an entire sample-loaded device was determined by analysing the measured data with complimentary simulation results. The frequency dependent phase-shift $\phi(\omega)$ between the sample and reference measurements was calculated, from which the effective permittivity increase was calculated and added to the permittivity of an air-filled channel ($\varepsilon_{\text{lut}} = 1$) as determined by HFSS. The effective permittivity of the entire device filled with an LUT is therefore

$$\varepsilon_{\text{eff}}(\omega, \varepsilon_{\text{lut}}) = \left(\frac{c\phi(\omega)}{\omega d} + \sqrt{\varepsilon_{\text{eff}}(\omega, 1)} \right)^2, \tag{1}$$

where d is the length of the transmission line.

The sample permittivity was found by interpolating the HFSS results shown in Fig. 1(b) for each sample measured. A range of monohydric alcohols (methanol, ethanol, propan-1-ol, butan-1-ol, hexan-1-ol, and octan-1-ol) and a dihydric alcohol (ethan-1,2-diol) were measured, and their permittivities calculated as shown in Fig. 2(a). The monohydric series of alcohols comprise alkanes in which a hydrogen atom has been replaced by a hydroxyl group, bound to the carbon atom indicated by the numerical prefix. The monohydric alcohols showed a systematic decrease in permittivity as the carbon chain length (and molecular weight accordingly) was increased, yet the dihydric alcohol exhibited a much greater permittivity.

The results were verified by comparison with the data provided in Ref. [6], in which deionised (DI)-H_2O, methanol, and propan-2-ol were measured in a free space THz-TDS system. A comparison between the data recorded from the on-chip solution presented here, and the results from Ref. [6] is shown in Fig. 2(b). The methanol and propan-2-ol data correlate strongly between the measurement techniques, however, there is a deviation in the calculated permittivity of DI-H_2O. This is because the radial Goubau mode illustrated in Fig. 1(a) has a cut-off frequency [7]

$$f_{\text{c}} = \frac{\text{c}}{h\sqrt{\varepsilon' + 1}}, \tag{2}$$

for an unloaded device, where h and ε' are the thickness and real permittivity of the substrate respectively. Above f_{c}, unwanted propagation modes become dominant as the substrate exhibits rectangular waveguide-like behaviour. In this state, the HFSS model and the performance of the practical device differ significantly, and the sample permittivity cannot be accurately determined above f_{c} without reducing the substrate thickness or channel depth, thereby increasing the cut-off frequency.

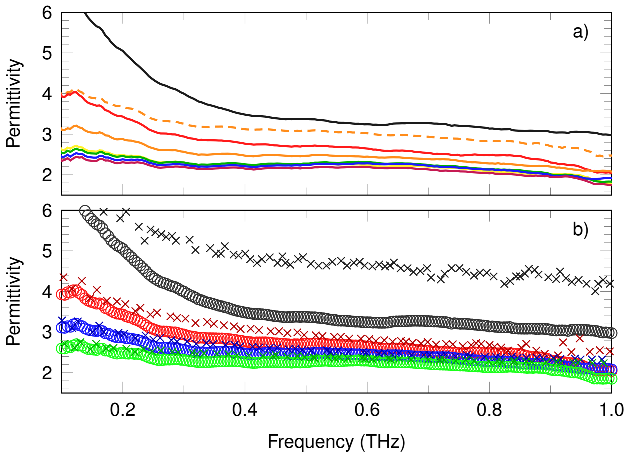

Fig. 2. a) The measured permittivity of DI-H_2O (black), ethan-1,2-diol (orange, dashed), methanol (red), ethanol (orange) propan-1-ol (yellow), butan-1-ol (green), hexan-1-ol (blue), and octan-1-ol (purple). b) The frequency-dependent permittivity of DI-H_2O (black), methanol (red), ethanol (blue) and propan-2-ol (green) as determined in this work (○), and by Ref. [6] (×).

III. CONCLUSION

We have demonstrated a method for the estimation of the permittivity of liquid samples in a microfluidic device using an integrated PGL terahertz waveguide. The fabricated structure was modelled in HFSS, and the calculated effective permittivity of the device for a range of dummy samples was used to determine the frequency-dependent permittivity of several LUTs. We anticipate this technique can be used to underpin future frequency-dependent analysis of data obtained using on-chip devices that cannot be solved analytically.

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