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A MICROWAVE METHOD FOR UNIQUE AND NON-AMBIGUOUS PERMITTIVITY DETERMINATION OF LIQUID MATERIALS FROM MEASURED UNCALIBRATED SCATTERING PARAMETERS

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Abstract—A new microwave method based on calibration-independent measurements has been proposed for non-ambiguous complex permittivity determination of liquid materials. We have derived a function in terms of the first-reflection coefficient of the sample using raw complex scattering parameter measurements of three measurement configurations. We have verified the proposed method from measurements of two liquid test samples with the available reference data in the literature.

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1. INTRODUCTION

Many microwave methods have been proposed for electrical characterization of different sort of materials [1–14]. These methods can roughly be divided into two groups as a) resonant methods and b) non-resonant methods [1]. Resonant methods have much better accuracy and sensitivity than non-resonant methods [1] at discrete frequencies and are applied to characterization of low-loss materials. On the other hand, non-resonant methods have relatively higher accuracy over a broad frequency band and necessitate less sample preparation compared to resonant methods [1].

Microwave non-resonant methods can also be separated into two groups as a) calibration-dependent methods and b) calibration-independent methods [15–26]. The advantages of methods in the latter group over those in the former one are that their accuracy can be improved by avoiding the usage of imperfect calibration-standards [22, 24] and that they reduce the overall measurement time. In order to analyze the accuracy of measurements and monitor the correctness of the extraction of electrical properties of materials, a metric function applicable to various calibration-independent methods has been derived for reflecting or non-reflecting measurement cells [27–29].

In calibration-independent methods, measurements of one sample [15–19, 21, 24, 26] are more attractive than those of two identical samples with different lengths [20, 22, 23, 25] for two reasons. First, they eliminate any impurity and/or inhomogeneity present in the second sample. Second, they decrease any thickness uncertainty that can arise from using the second sample.

There is a need to study the interaction of electromagnetic waves with living organisms and their effects on biological materials for evaluation of any possible health hazards and non-thermal effects to the human-being and environment. The amount of energy absorbed is a function of the relative complex permittivity (ε_r) of a material [1]. Therefore, it is important to know the dielectric properties of biological materials and thus their various constituents [30–34]. In addition, accurate ε_r determination of liquid materials at microwave frequencies is necessary for applications such as the evaluation of biological effects in biological molecules and in solvents [30].

In the literature, various calibration-independent methods have been proposed for electrical characterization of liquid materials [18–20]. Although they are attractive in measuring accurate ε_r of these materials, they necessitate a pre-knowledge of the range of possible ε_r since they result in two eigen values. To resolve this problem,

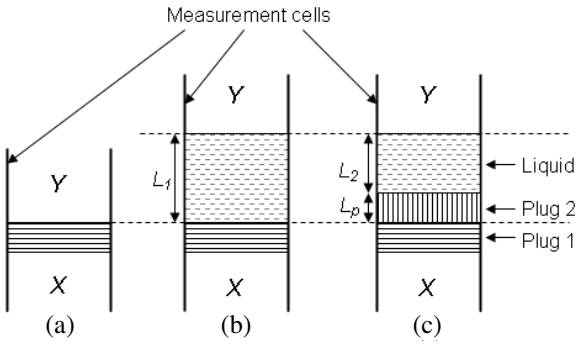

Figure 1. Measurement configurations for permittivity extraction of liquid materials using uncalibrated scattering parameter measurements from a VNA.

a simple technique using the comparison of eigen values at different frequencies was introduced [35]. In applying this technique, for the first two lowest frequencies in the band, the positive solution of eigen values is arbitrarily retained and plotted in the complex plane. For each of next frequencies, the two possible solutions of eigen values are tested and only the one which ensures a monotonous variation in the complex plane is taken as the correct solution. This technique resembles to the technique developed by Weir for choosing the correct constitutive parameters among multiple solutions by comparing measured and calculated group delays at two closely separated frequencies [10]. Also, it is similar to that we recently developed for determining unique ε_r of medium- and low-loss materials using amplitude-only scattering (S-) parameter measurements at slightly separated frequencies [8, 36, 37]. Although the technique in [35] is effective in finding one solution for eigen values and ε_r thereof, it may not be suitable for dispersive materials. Any method which is applicable to wide range of materials can find wide applications in the literature. The motivation of this research paper is to propose a calibration-independent microwave method for accurate and unique ε_r inversion of liquid materials. The method works very well in limited frequency-band applications or for dispersive materials since it is based upon point-by-point or (frequency-by-frequency) measurements.

2. MODEL FOR THE PROBLEM

We consider the measurement configurations shown in Fig. 1 for ε_r inversion of liquid materials. While Fig. 1(a) illustrates the empty

cell (no liquid sample) connection, Figs. 1(b) and 1(c) show the measurement configurations where the liquid sample with length L_1 is poured onto a dielectric plug (Plug 1) and where the liquid sample with length L_2 is poured onto another dielectric plug (Plug 2) with length L_p.

The two ports referred to as X and Y in Fig. 1 are used as transitions between a vector network analyzer (VNA) and the configurations in Figs. 1(a)–1(c). These ports include source and load match errors, tracking errors, hardware imperfection of VNA [15–19]. It is assumed that X and Y are unequal and are unchanged for each configuration in Fig. 1.

A microwave network with an arbitrary number of ports can be characterized by using S-parameter presentation. However, in practice, many microwave networks consist of a cascade connection of two or more two-port networks (e.g., X and Y in Fig. 1). In these circumstances, it is convenient to use ABCD matrix [21, 38, 39] or wave cascading matrix (WCM) presentations [40] of such microwave networks. For the mathematical analysis in this paper, we utilize the wave cascading matrix (WCM) since it is useful in calibration/error correction problems [22, 24]. We denote the two-port WCM matrices, T_X, T_Y, T_{P_1}, T_{P_2}, T_{L_1} and T_{L_2}, respectively, for modeling the transitions X and Y, Plugs 1 and 2 and the liquid samples with lengths L_1 and L_2. For each of these ports, we can write their theoretical expressions for the derivation of ε_r. Since our method eliminates the need for knowledge of T_X, T_Y and T_{P_1}, we will only deal with T_{P_2}, T_{L_1} and T_{L_2} for ε_r determination. The expressions for these ports can be obtained by finding electric fields in each port, which can be derived from their vector potentials $\vec{A}$ and $\vec{F}$ [41] (or Hertzian vectors) as

$$\vec{E}^{(n)} = -j\left[\omega\vec{A}^{(n)} + \frac{1}{\omega\mu_{(n)}\varepsilon_{(n)}}\nabla\left(\nabla\cdot\vec{A}^{(n)}\right)\right] - \frac{1}{\varepsilon_{(n)}}\nabla\times\vec{F}^{(n)}, \quad (1)$$

where n signifies each different medium between X and Y in Fig. 1 and $n = P_2, L_1$ and L_2. The magnetic fields corresponding to the electric fields in (1) can be found by the duality of electromagnetic fields [41].

Assuming that the rectangular waveguide operates in the dominant mode (TE_{10}) and that the sample has a flat surface and there is no air gap between the sample external surfaces and inner waveguide walls, we have $\vec{A}^{(n)} = 0$ and $\partial F_z^{(n)}/\partial y = 0$ [41]. Then, the electric vector potential can be written for each two port network in Fig. 1 as

$$F_z^{(n)}(x,z) = \cos\left(\frac{2\pi}{\lambda_c}x\right)\left[C_{1n}e^{-\gamma_n z} + C_{2n}e^{\gamma_n z}\right], \quad (2)$$

where

$$\gamma_n = j\left(2\pi/\lambda_0\right)\sqrt{\varepsilon_{(n)}\mu_{(n)} - \lambda_0^2/\lambda_c^2}. \tag{3}$$

Here, C_{1n} and C_{2n} are constants (reel or complex); $\lambda_0 = c/f$ and $\lambda_c = c/f_c$ correspond to the free-space and cut-off wavelengths; f, f_c, and c are, respectively, the operating and cut-off frequencies and the speed of light; and $\varepsilon_{(n)} = \varepsilon'_{(n)} - j\varepsilon''_{(n)}$ and $\mu_{(n)} = \mu'_{(n)} - j\mu''_{(n)}$ are the complex permittivity and complex permeability of each medium between X and Y.

Using the electric vector potentials in (2), electric and magnetic fields can be determined from (1) using duality for each medium [41]. Here, we assume that the measurement cells in Fig. 1 are homogenous, isotropic and non-reflecting and that the Plug 2 and the sample are homogenous and isotropic. Applying boundary conditions (continual of electric and magnetic fields at each region interface), S-parameters for each region can be derived [16]. As a result, we can write the WCM matrices for Plug 2 and sample with lengths L_1 and L_2 as

$$T_{Lk} = \frac{1}{\left(1-\Gamma^2\right)T_k}\begin{bmatrix} T_k^2 - \Gamma^2 & \Gamma\left(1-T_k^2\right) \\ -\Gamma\left(1-T_k^2\right) & 1-\Gamma^2 T_k^2 \end{bmatrix}, \quad \begin{matrix} k=1,2 \\ T_k = e^{-\gamma L_k} \end{matrix}, \tag{4}$$

$$T_{P_2} = \frac{1}{\left(1-\Gamma_p^2\right)T_p}\begin{bmatrix} T_p^2 - \Gamma_p^2 & \Gamma_p\left(1-T_p^2\right) \\ -\Gamma_p\left(1-T_p^2\right) & 1-\Gamma_p^2 T_p^2 \end{bmatrix} = \begin{bmatrix} \Lambda_1 & \Lambda_2 \\ -\Lambda_2 & \Lambda_3 \end{bmatrix}, \tag{5}$$

where

$$\begin{aligned} &\Gamma = -\frac{\gamma-\gamma_0}{\gamma+\gamma_0},\ T_k = \exp\left(-\gamma L_k\right),\ k=1,2, \\ &\Gamma_p = -\frac{\gamma_p-\gamma_0}{\gamma_p+\gamma_0},\ T_p = \exp\left(-\gamma_p L_p\right), \end{aligned} \tag{6}$$

$$\begin{aligned} &\gamma_0 = j\frac{2\pi}{\lambda_0}\sqrt{1-\lambda_0^2/\lambda_c^2},\ \gamma = j\frac{2\pi}{\lambda_0}\sqrt{\varepsilon_r - \lambda_0^2/\lambda_c^2}, \\ &\gamma_p = j\frac{2\pi}{\lambda_0}\sqrt{\varepsilon_{pr} - \lambda_0^2/\lambda_c^2}, \end{aligned} \tag{7}$$

where γ_0, γ and γ_p represent, respectively, the propagation constants of the air-filled, sample-filled and plug-filled (Plug 2) regions in the cell; L_1, L_2 and L_p are, respectively, the lengths of identical liquid samples and of Plug 2 inside the cell; Γ, Γ_p, T and T_p are the first reflection and transmission coefficients of the sample and Plug 2; and $\varepsilon_r = \varepsilon'_r - j\varepsilon''_r$ and $\varepsilon_{pr} = \varepsilon'_{pr} - j\varepsilon''_{pr}$ are the relative complex permittivities of the liquid sample and Plug 2.

Whole WCM matrices of each configuration in Fig. 1 can be written as

$$M_a = T_X T_{P_1} T_Y,\ M_b = T_X T_{P_1} T_{L_1} T_Y,\ M_c = T_X T_{P_1} T_{P_2} T_{L_2} T_Y, \tag{8}$$

where

$$M_i = \frac{1}{S_{21_i}} \begin{bmatrix} (S_{12_i}S_{21_i} - S_{11_i}S_{22_i}) & S_{11_i} \\ -S_{22_i} & 1 \end{bmatrix}, \; i = a, b, c, \tag{9}$$

and S_{km} parameters $(k, m = 1, 2)$ are measured raw S-parameters and subscripts 'a', 'b' and 'c' in (8) and (9), respectively, correspond to the measurement configurations in Figs. 1(a)–1(c).

3. UNIQUE PERMITTIVITY DETERMINATION

In the theoretical analysis, it is assumed that the electrical and physical properties of Plug 2 in Fig. 1 are known. Using the WCM matrices in (8) and (9), we show that it is possible to non-ambiguously inverse the ε_r from the measurement configurations in Fig. 1. To this end, we firstly eliminate T_Y from (8) as

$$M_b M_a^{-1} = T_X T_{P_1} T_{L_1} T_{P_1}^{-1} T_X^{-1}, \; M_c M_b^{-1} = T_X T_{P_1} T_{P_2} T_{L_2} T_{L_1}^{-1} T_{P_1}^{-1} T_X^{-1}, \tag{10}$$

where '$\cdot$'$^{-1}$ means the inverse of a square matrix '$\cdot$'. So as to eliminate the dependence of $M_b M_a^{-1}$ and $M_c M_b^{-1}$ on T_{P_1} and T_X, we note from (10) that $M_b M_a^{-1}$ and T_{L_1}, and $M_c M_b^{-1}$ and $T_{P_2} T_{L_2} T_{L_1}^{-1}$ are similar matrices. It is well known that similar matrices have the same trace (denoted by Tr) which takes the summation of diagonal elements in a square matrix [16]. As a result, from (10), we find

$$Tr\left(M_b M_a^{-1}\right) = Tr\left(T_{L_1}\right), \; Tr\left(M_c M_b^{-1}\right) = Tr\left(T_{P_2} T_{L_2} T_{L_1}^{-1}\right). \tag{11}$$

Using (4), (5) and (11), we obtain

$$Tr\left(T_{L_1}\right) = T_1 + 1/T_1, \tag{12}$$

$$Tr\left(M_c M_b^{-1}\right) = \frac{2\Lambda_2\Gamma\left(1 - (T_1/T_2)^2\right) + \Lambda_1\left(1 - \Gamma^2 (T_1/T_2)^2\right) + \Lambda_3\left((T_1/T_2)^2 - \Gamma^2\right)}{(1-\Gamma^2)(T_1/T_2)}. \tag{13}$$

It is obvious from (12) that there are two eigen values (denoted by T_1 in (12)) and it is not clear which one is for travelling waves to the left and vice versa [35]. In order to resolve this ambiguity, a simple technique based upon the comparison of T_1 values at different frequencies was proposed. However, this technique may not be suitable either for dispersive materials or ε_r measurements in limited frequency-band applications. In addition, assuming that T_1 is non-ambiguously measured by [35], there are still multiple solutions for ε_r from the measured T_1 [9]. A pre-estimate value for ε_r can be used as a solution to this problem. However, it is not possible to know the electrical

properties of some newly investigated materials. Therefore, a method should be proposed to resolve these two problems simultaneously.

In this research paper, we utilize two-independent T_1 measurements at one frequency as a remedy to the problems discussed above. We derive a metric function in terms of only Γ for unique and accurate ε_r inversion at one-frequency. To this end, firstly, we express T_1/T_2 in terms of $Tr\left(T_{L_1}\right)$ as

$$T_{1(1,2)} = Tr\left(T_{L_1}\right)/2 \mp \sqrt{\left[Tr\left(T_{L_1}\right)/2\right]^2 - 1},\ T_1 \Big/ T_2 = T_1^{(1-L_2/L_1)}. \quad (14)$$

Then, substituting (14) into (13), we obtain a function in terms of Γ as

$$\Gamma_{(1,2)} = -\alpha_0 \mp \sqrt{\alpha_0^2 - \alpha_1},$$

$$\alpha_0 = \frac{\Lambda_2\left(1 - (T_1/T_2)^2\right)}{Tr\left(M_c M_b^{-1}\right)(T_1/T_2) - \Lambda_1\left(T_1/T_2\right)^2 - \Lambda_3}, \quad (15)$$

$$\alpha_1 = \frac{\Lambda_1 + \Lambda_3\left(T_1/T_2\right)^2 - Tr\left(M_c M_b^{-1}\right)(T_1/T_2)}{Tr\left(M_c M_b^{-1}\right)(T_1/T_2) - \Lambda_1\left(T_1/T_2\right)^2 - \Lambda_3}. \quad (16)$$

In the selection of the correct root from (15), we use the constrain $|\Gamma| \leq 1$. Finally, using (16), the ε_r of the sample can be determined as

$$\varepsilon_r = \lambda_0^2/\lambda_c^2 + \left(1 - \lambda_0^2/\lambda_c^2\right)\frac{(1-\Gamma)^2}{(1-\Gamma)^2}. \quad (17)$$

The importance of the derivation in (14)–(17) is two-folds. First, it does not have any T_1 and T_2 terms. Second, it eliminates the possibility of producing multiple solutions for ε_r thereof.

4. MEASUREMENTS

We constructed a simple waveguide set-up operating at X-band to measure the ε_r of liquid materials [8]. A HP8720C VNA is connected as a source and measurement equipment. It has a 1 Hz frequency resolution (with option 001) and 8 ppm (parts per million) frequency accuracy. Waveguide sections have a width of $22.86 \mp 5\%$ mm ($f_c \cong 6.555$ GHz). Two waveguide sections with lengths ($70 \mp 5\%$ mm) greater than two free-space wavelengths are used between the sample holder (waveguide section) and coaxial-to-waveguide adapters to filter out any higher order modes.

We machined two identical polytetrafluoro-ethylene (PTFE) samples with different lengths (L_p = 3 mm for Plug 2 and 10 mm

for Plug 1) as for dielectric plugs in Fig. 1. Since their electrical properties do not considerably change with frequency, we assume that their ε_r stay approximately constant ($\varepsilon_r \cong 2.05 - j0.0014$) over 8.2–12.4 GHz frequency range (X-band) [14]. We used two test liquid samples (distilled water and methanol) for validation of the proposed method. In the application of our method, firstly we positioned the longer plug into a 76.28 mm long waveguide section (measurement cell) and measured the raw scattering parameters of this configuration (Fig. 1(a)). As a second step, we poured some test sample onto the longer plug and arranged its length to 7 mm using a high-precision micrometer. Then, we measured the raw scattering parameters of this configuration (Fig. 1(b)). Next, we took whole test sample out and waited sometime for drying the inner of cell. After that, we positioned the shorter plug over the longer one and then poured the same test sample onto it. We set the length of the test sample to 4 mm using the micrometer and measured the uncalibrated scattering parameters of this last configuration (Fig. 1(c)). Finally, we extracted the ε_r of the test samples using (15)–(17). Figs. 2 and 3 demonstrate the measured ε_r of distilled water and methanol by the proposed method.

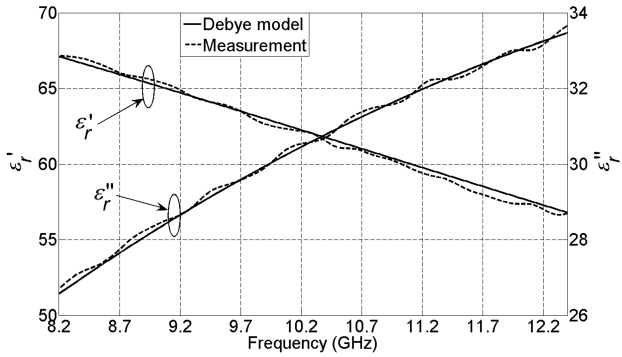

Figure 2. Measured (dashed line) and theoretical (solid line) ε_r of distilled water over X band. The parameters for the Debye model are $\varepsilon_\infty = 5.2$, $\varepsilon_s = 78.5$ and the relaxation time $\tau = 8.3$ ps at ordinary room temperature [43].

It is seen from Figs. 2 and 3 that the measured ε_r of distilled water and methanol are completely in good agreement with those obtained from the theory (the Debye model) [43, 44]. The advantages of the proposed method over those in [18–20] and [35] are that it does not require any initial guess or knowledge of the ε_r and is applicable to dispersive materials or suitable for limited frequency-band applications. It should be pointed out that the proposed method

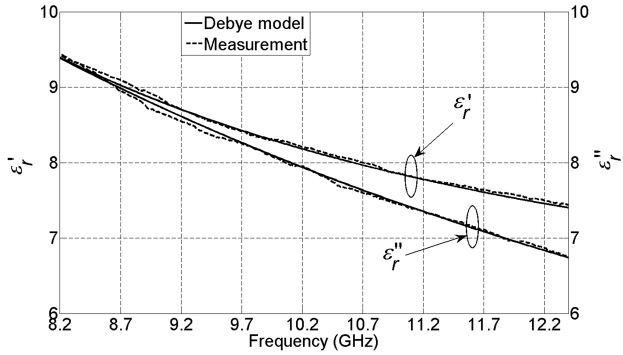

Figure 3. Measured (dashed line) and theoretical (solid line) ε_r of methanol over X band. The parameters for the Debye model are $\varepsilon_\infty = 5.6$, $\varepsilon_s = 32.6$ and the relaxation time $\tau = 48\,\text{ps}$ at ordinary room temperature [44].

is not applicable for either non-uniform cells [45, 46] or anisotropic materials [47].

5. CONCLUSION

A microwave method has been proposed for non-ambiguous complex permittivity determination of liquid materials from measured uncalibrated scattering parameters. The method uses two-independent measurements of eigen values for unique permittivity determination at one-frequency. We have validated the proposed method from measurements of two test samples with their reference data in the literature. It is shown that they are in good agreement with those in the literature.

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