Material Parameter Extraction in THz Domain, Simplifications and Sensitivity Analysis

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Abstract—Classic equations for material parameter extraction are reconsidered and slightly modified to achieve stable results at all frequencies. Meanwhile, closed-form solutions are developed to simplify the material parameter extraction process and uncertainty evaluation. The presented equations are independent of the material-slab thickness and therefore, can reduce the relevant systematic errors and uncertainties. Some representative results are reported in the frequency range 140-220 GHz together with the uncertainty analysis and sensitivity coefficients.

Keywords—material characterization, extraction method, THz domain, sensitivity coefficient, measurement uncertainty

I. INTRODUCTION

Material parameter-extraction methods are based on reflection and transmission parameters (or only one of them) that often suffer from instability or complicated iterative process. The classic Nicolson-Ross-Weir (NRW) method [1] deals with Γ and T (see Eq.1 and Eq.2, for free-space propagation) to extract μ and ϵ , simultaneously. The method gives unstable results for low-loss and high-refractive materials when $S_{11} \sim 0$ and $|S_{21}| \sim 1$ at specific frequencies.

$$S_{11} = \frac{\Gamma(1-T^2)}{1-\Gamma^2 T^2} \quad S_{21} = \frac{T(1-\Gamma^2)}{1-\Gamma^2 T^2} \quad (1)$$

$$\rightarrow \Gamma = X \pm (\sqrt{X^2 - 1}) \quad \text{and} \quad \frac{\epsilon_r}{\mu_r} = \left(\frac{1-\Gamma}{1+\Gamma}\right)^2 \quad (2)$$

with: $X = (S_{21}^2 - S_{11}^2 + 1) / 2S_{11}$

$$T = e^{-j\frac{\omega}{c}d\sqrt{\mu_r\epsilon_r}} \quad (3)$$

Here, a simple comprehensive method is suggested to correct the instability first, and then classic equations (1 and 2) are simplified to closed-form formula.

II. INSTABILITY CORRECTION

In the NRW method [1], [2] the extraction (μ and ϵ) is established on Eq.1 together with $\text{Ln}(T)$ -complex function- in Eq.3 and treating its phase ambiguity. Although the method has instability at some frequencies, but T and consequently $\sqrt{\mu_r\epsilon_r}$ are stable.

The correction method here is based on the fact that in NRW method the unstable ϵ and μ are extracted in parallel, and their product is stable:

$$\epsilon(\text{unstable}) \times \mu(\text{unstable}) = \epsilon(\text{stable}) \times \mu(\text{stable})$$

Therefore, in the case of non-magnetic materials for which $\mu_r = 1 + j0$, the correction factor is derived as simple as:

$$\epsilon(\text{stable}) = \epsilon(\text{unstable}) \times \mu(\text{unstable}) \quad (4)$$

In which $\epsilon_r(\text{unstable})$ and $\mu_r(\text{unstable})$ can be determined from the well-known algorithms based on the NRW method. Simply saying, the unstable $\mu = \mu' + j\mu''$ (deviated from $1 + j0$) is used as the correction factor.

Fig. 1. 3mm Plexiglass slab (140-220 GHz): ϵ_r Real (top) and Imaginary parts, stable results compared with unstable ones with "unstable $\mu = \mu' + j\mu''$ " as the correction factor (black curves, bottom).

Figure 1 shows the results for a 3mm Plexiglass slab measured with quasi-TEM free-space techniques [3] in the frequency-range 140-220 GHz. The hardware itself should be calibrated to give the S-parameters (both reflection and transmission) on the material surface after an adequate full two-port calibration of the Vector Network Analyzer (VNA). METAS VNA-Tools II [4] has been used to show the extracted material parameters with classic methods. VNA-Tools is a metrology software to compute uncertainties of the measured S-parameters with various post-processing features including material parameter extraction with associated uncertainties. This correction process can be extended to the other type of materials if μ or ϵ is known for some single frequencies or frequency-ranges.

Free-space propagation conditions, setup limits and the multi-step calibration process of the measurement setup (VNA + quasi-TEM hardware) are crucial points for the reliability of the final results. This is out of the scope of the present paper.

III. SIMPLIFICATIONS AND SENSITIVITY ANALYSIS

Here, the classic equations (1), (2) which relate the S-parameters to Γ and T are simplified to closed-form.

$$\frac{\epsilon_r}{\mu_r} = \left(\frac{1-\Gamma}{1+\Gamma} \right)^2 = \left(\frac{(1-X) \mp \sqrt{X^2-1}}{(1+X) \pm \sqrt{X^2-1}} \right)^2 \quad (5)$$

Some developments on Eq.5 lead to:

$$\frac{\epsilon_r}{\mu_r} = \left(\frac{(1-X) \mp \sqrt{X^2-1}}{(1+X) \pm \sqrt{X^2-1}} \right)^2 = \frac{(X-1)(X \pm \sqrt{X^2-1})}{(X+1)(X \pm \sqrt{X^2-1})} \rightarrow$$

$$\frac{\epsilon_r}{\mu_r} = \frac{X-1}{X+1} = \frac{(S_{11}-1)^2 - S_{21}^2}{(S_{11}+1)^2 - S_{21}^2} \quad (6)$$

Equation (6) is independent of the material thickness and can give reliable and stable results if S_{11} is not very small. Yet, the instability problems appear for low-loss materials when $S_{11} \sim 0$ and $|S_{21}| \sim 1$ at specific frequencies the same as in the classic NRW method [1], [2]. Similar relations have been already used to determine the impedance of transmission lines with dielectric filled sections [5].

Closed-form Eq.6 could provide a more comprehensive analysis of the uncertainties with clear contribution of each measured S-parameter.

The measurement results and extracted parameters cannot be reliable without a comprehensive error analysis and establishing the associated uncertainties. By applying the partial derivatives of Eq.6, sensitivity coefficients of epsilon can be derived as a function of S_{11} and S_{21} . Simple and closed-form structure of Eq.6 makes its derivatives closed-form, as well.

$$\frac{\partial \epsilon_r}{\partial S_{11}} = \frac{4(S_{11}^2 + S_{21}^2 - 1)}{\{(S_{11}+1)^2 - S_{21}^2\}^2}$$

$$\frac{\partial \epsilon_r}{\partial S_{21}} = \frac{-8 S_{11} S_{21}}{\{(S_{11}+1)^2 - S_{21}^2\}^2} \quad (7)$$

Figure 2 shows the sensitivity coefficients of the permittivity for the sample of Fig.1. As shown, for both S_{11} and S_{21} there are nearly simultaneous minimum sensitivity points which are in agreement with the results of "instability corrected" curves in Fig.1. Given nominal $|\Delta S_{11}|$ and $|\Delta S_{21}|$ about 0.015, the associated uncertainty of $|\epsilon_r|$ is estimated around 0.1 when $\epsilon'_r = 2.6$. Therefore, the simple closed-form (yet unstable) Eq.6 can give reliable results with calculable uncertainties around the frequencies: 140GHz, 170GHz and 200GHz (Fig.1 and Fig. 2).

Fig. 2. 3mm Plexiglass slab, sensitivity coefficients of ϵ_r (140-220 GHz): unstable ϵ_r Real (blue), and sensitivity coefficients of S_{11} and S_{21} .

Actually, reliable results of ϵ'_r (real part) even for a limited number of points in a given frequency-range is of interest. Most of the "normal" homogeneous materials have nearly constant ϵ_r in mm-Wave/sub-THz domain. Besides, the calculation of ϵ_r and its associated uncertainties is independent of the slab thickness. The thickness of the slab and its positioning can be one of the major uncertainty contributions (cause systematic error) in reflection-and-transmission methods [2] and transmission-only methods [6], as well.

It can be shown the ϵ_r uncertainty minimum points occur when the measured $|S_{11}|$ and $|S_{21}|$ reach their Max. and Min. (Fabry-Perot multiple-reflection inside the slab), consequently. This fact may still make the extraction and uncertainty evaluation process easier.

As mentioned, closed-form Eq.6 is independent of the slab's thickness and can correct the systematic errors caused by this sensitive parameter. Fig.3. shows the high sensitivity of the extracted ϵ'_r (real part) of a 2mm (nominal thickness) fused-Silica "F.Si" slab. The parameter extracted by non-iterative stable method [2] varies about 5%, which is a considerable systematic error. This is regarding $\epsilon'_r = 4.05$ (for nominal 2mm thickness), to $\epsilon'_r = 3.9$ (2.04mm thickness, measured with high precision mechanical devices) and finally $\epsilon'_r = 3.8$ (for 2.07mm thickness, which gives reasonable match to Eq.6. at the best uncertainty points: ~167GHz and ~205GHz)

Fig. 3. 2mm F.Si slab, ϵ_r' and sensitivity coefficients of ϵ_r' (140-220 GHz). Extracted ϵ_r' with thicknesses 2.00mm (top-left), 2.04mm (top-right) and 2.07mm (bottom-right). Non-iterative stable method [2] (black) and Eq.6. (red) are used, optimal match ($\epsilon_r' \approx 3.8$) with 2.07mm thickness at the "best" uncertainty points: $\sim 167\text{GHz}$ and $\sim 205\text{GHz}$.

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