

Estimation methods to extract complex permittivity from transmission coefficient in the terahertz band

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Abstract

In this paper, the characteristics of the transmission coefficient (S_{21}) measured in free-space at terahertz frequencies are analyzed. The analysis results are used to estimate the permittivity of the material under test, and the estimated permittivity is adopted as an initial-value for the iterative algorithm to extract the complex permittivity of the material from the S_{21} . The iterative extraction technique based on the estimation is efficient, while the iterative extraction technique without the estimation is inefficient. Various known materials in the literature are used to validate the technique in the terahertz band.

Keywords Complex permittivity · Terahertz · Free-space · Initial-guess

1 Introduction

Measurements of relative complex permittivity (ϵ_r) in the terahertz (THz) band are required for engineering designs of THz devices (e.g., lenses, waveguide, filters, etc.) (Hammler et al. 2016; Sahin et al. 2018a; Kazemipour et al. 2015; Yang et al. 2019; Güneşer 2019; Ali et al. 2017; Moradiani et al. 2020; Farmani et al. 2020). Free-space techniques have been widely used for dielectric characterization at THz frequencies, particularly since recent advances in THz components and instrumentation have made them more convenient and accurate (Zhang et al. 2017; Sahin et al. 2018b; Tosaka et al. 2015; Ghalichechian

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and Sertel 2015). The advances in the THz measurement can be summarized as two parts: (1) the gate-reflect-line (GRL) calibration technique and lens are used for the measurement system to improve the accuracy of the measurements (Zhang et al. 2017); (2) the environment of the calibration and the measurement is set to be clear to remove the impact of water vapor and O2 absorption lines (Sahin et al. 2018b), that also improve the accuracy of the measurements. However, the reflection coefficient (S_{11}) of the material under test (MUT) is still hard to be measured above 300 GHz (Kazemipour et al. 2015; Lamb 1996). Since only the transmission coefficient (S_{21}) can be used for the characterization above 300 GHz, the ε_r of the MUT needs be extracted by the iterative algorithms.

But the iterative extraction techniques (e.g., Newtons method) restrict the application of the free-space transmission techniques, because the convergent values of the extracted ε_r vary with the initial guesses for the iterative extraction techniques (see Fig. 5 in Zhang et al. 2017). Some publications simply ignored the problem on multiple convergent values (see Hammler et al. 2016; Sahin et al. 2018b; Tosaka et al. 2015), some experimentally reported the phenomena of getting multiple results and proposed method to obtain a right initial value by using S_{11} and S_{21} (Yang et al. 2019; Zhang et al. 2017), though S_{11} is hard to be measured. While in Ghalichechian and Sertel (2015) technique without detailed analysis was proposed to estimate permittivity from S_{21} in Zhang et al. (2017). But the technique fails to work when the electrical length of the MUT is large. In addition, the empirical value at low frequency of the MUT was adopted as the initial value for the iterative techniques to extract the ε_r in the THz band (Ghalichechian and Sertel 2015). If there is a new material or the value of the ε_r of the MUT in the THz band is much different from the value at low frequencies (see Fig. 10 in Seiler and Plettemeier (2019)). The extracted value of the permittivity is incorrect if the estimated value is far away from the true value (Yang et al. 2019). How to get a right initial-guess for the iterative extraction techniques is still an open-question.

In this paper, the proper initial-value for the iterative extraction techniques is estimated by using the properties of the measured S_{21} in the THz band. The availability of the proposed technique is verified by various known materials (e.g. PMMA, PVC, Teflon, Glass, Crosslinked SUEX, etc.) in the THz-band.

2 Theory and technique

A schematic of a MUT with thickness of t is shown in Fig.1. The MUT is measured in freespace. According to the analytical multilayer transmission model, transmission through a dielectric slab with thickness t can be expressed as Farmani et al. (2020)

$$S_{21} = \frac{4\sqrt{\varepsilon_r}e^{-j\omega\sqrt{\mu_0\varepsilon_0}\sqrt{\varepsilon_r t}}}{(1+\sqrt{\varepsilon_r})^2 - (1-\sqrt{\varepsilon_r})^2 e^{-j2\omega\sqrt{\mu_0\varepsilon_0}\sqrt{\varepsilon_r t}}}$$
(1)

where $\varepsilon_r = \varepsilon'_r - j\varepsilon''_r$ is the relative complex permittivity of the MUT, ω is the angular frequency, and *t* is outside of the square.

If the thickness of the MUT is larger than one or more wavelengths, the S_{21} changes periodically with the frequency (Hammler et al. 2016). In the THz band, the wavelengths of the electromagnetic waves are short that the thickness of the MUT can be longer than one or more wavelengths. In this work, we estimate the permittivity of the MUT from the S_{21} by using the special properties.



Fig. 1 A schematic of a MUT measured in free-space

2.1 Method 1: using properties of |S₂₁|

For low-loss materials, when the thickness of the MUT is an integer multiple of halfwavelength $(\lambda/2)$ inside the MUT, there is a sharp peak in the measured $|S_{21}|$ due to Fabry CPerot effects (Ghalichechian and Sertel 2015). When there are two peaks in the measured $|S_{21}|$ and the MUT is non-dispersive or weakly dispersive between the two peak frequencies, the phase constants at the two frequencies can be derived as

$$\beta_1 = n\pi/t \tag{2}$$

$$\beta_2 = (n+1)\pi/t \tag{3}$$

where n is a positive integer.

As $(\alpha + j\beta)^2 = -\omega^2 \mu_0 \epsilon_0 (\epsilon'_r - j\epsilon''_r)$ and loss constant α is approximately equal to zero for low-loss materials, we can derive

$$\beta^2 \approx \omega^2 \mu_0 \varepsilon_0 \varepsilon'_r \tag{4}$$

Combining Eqs. (2)–(4), the permittivity between the two peak frequencies of the MUT can be estimated as

$$\varepsilon_r' \approx \left(\frac{1}{2t\sqrt{\varepsilon_0\mu_0}\Delta f_1}\right)^2 \tag{5}$$

where Δf_1 is the difference between the two peak frequencies.

2.2 Method 2: using properties of S₂₁

The method 1 is efficient when there are two or more peaks in the $|S_{21}|$. However, the peaks are not obvious when the MUT is thick as shown in Sahin et al. (2019). Because, the loss increases with the thickness, the resonance decreases with the loss. The difference between the peak and regular values is small. Therefore, we cannot use Eq. (5) for ε'_r estimation when the MUT is thick.

For the thick MUT, there are more frequencies where t is an integer multiple of wavelength inside the MUT. For the MUT with low loss tangent, the Eq. (1) can be approximately expressed as

$$S_{21} \approx \frac{4\sqrt{\epsilon_r'}e^{-j\omega\sqrt{\mu_0\epsilon_0}\sqrt{\epsilon_r'}t}}{(1+\sqrt{\epsilon_r'})^2 - (1-\sqrt{\epsilon_r'})^2e^{-j2\omega\sqrt{\mu_0\epsilon_0}\sqrt{\epsilon_r'}t}}$$
(6)

As seen in Eq. (6), the $\angle S_{21}$ is approximately 180° when the thickness of the MUT is an integer multiple of wavelength inside the MUT. We processed the two $|S_{21}|$ at two frequencies where $\angle S_{21}$ are equal 180°, the permittivity of the MUT can be estimated as

$$\varepsilon_r' \approx \left(\frac{1}{t\sqrt{\varepsilon_0\mu_0}\Delta f_2}\right)^2 \tag{7}$$

where Δf_2 is the difference between the two frequencies.

2.3 Application procedures of the two methods

The application procedures of the proposed methods are shown as follows:

Step 1: choose the method according to the characteristics of the S_{21} . If the number of the peaks in the $|S_{21}|$ is more than the number of the frequencies where the values of $\angle S_{21}$ are equal to 180°, the method 1 is chosen. Otherwise, the method 2 is chosen.

Step 2: determine the dispersion characteristics of the MUT. If all Δf_1 (or Δf_2) are approximate for the MUT, the MUT is non-dispersive over the entire measured frequency range. Otherwise, the MUT is dispersive over the entire measured frequency range.

Step 3.1: for the MUT which is non-dispersive over the entire measured frequency range, the average value of the Δf_1 (or Δf_2) is used for the permittivity estimation.

Step 3.2: for the MUT which is dispersive over the entire measured frequency range, the value of the Δf_1 (or Δf_2) is used for the permittivity estimation between the two adjacent frequencies. We can see that Δf would be used for different frequency band. If the materials whose permittivity change dramatically with frequency are measured, we should make them thick enough, that the permittivity between the Δf changes a little. Then the proposed can be efficient.

Step 4: Newtons method with the estimated initial value (permittivity) is performed.

3 Examples and discussion

3.1 The non- or weak dispersive samples in the literature

To validate the proposed technique, the $|S_{21}|$ in the figures of Hammler et al. (2016), Kazemipour et al. (2015), Sahin et al. (2018b) and Bourreau et al. (2006) are used for determining the Δf . We obtained the peak frequencies of the $|S_{21}|$ and processed the frequencies by Eq. (4). In theoretical, the values of the $|S_{21}|$ and the $|S_{21}|$ are equal to each other. The permittivity calculated by Eq. (5) agrees well with the extracted values in the literature as show in Table 1. The error between the calculated values and the values in the

Table 1 Com	parison of extracte	ed values with literature values				
Material	Equipment	Measured $ S_{21} $	Frequency (GHz)	ε'_r	Estimated error (%)	Source
HR-Si	NNA	From Hammler et al. (2016)	925	11.57	. 1	Hammler et al. (2016)
			750-1100	11.61	0.36	This work
PMMA	VNA	From Kazemipour et al. (2015)	300	2.595	I	Kazemipour et al. (2015)
			220-325	2.46	5.20	This work
PVC	VNA	From Seiler and Plettemeier (2019)	75-110	2.932	I	Seiler and Plettemeier (2019)
			75-110	2.892	1.36	This work
Uncured	TDS	From Moradiani et al. (2020)	90-2000	2.91 - 3.08	I	Moradiani et al. (2020)
SUEX			90-2000	2.93	0.67-4.87	This work

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literature ranges from 0.36 to 5.20%. However, the phase angles of the S_{21} are not presented in Kazemipour et al. (2015), Sahin et al. (2018b) and Bourreau et al. (2006). We cannot determine the ε_r over the entire measured frequency range by using the Newtons method.

In this work, we used the extracted in Kazemipour et al. (2015) and Sahin et al. (2018b) to simulate the S_{21} in the THz band. The ε_r of the materials are put into Eq. (1). The simulation method is shown in Seiler and Plettemeier (2019). The simulated S-parameters are calculated using the values of ε_r (Bourreau et al. 2006). That is reasonable, because the measured and simulated S21 in free-space at THz frequencies are almost the same (see Fig. 6 in Bourreau et al. (2006)). In our previous work, *S*-parameters simulated in the THz band have been further proved for validating extraction techniques (Yang et al. 2019).

Since the measurable frequency range is different when using a vector network analyzer (VNA) and by TDS (time-domain spectroscopy) (Tosaka et al. 2015), PMMA, PVC, Teflon, Plexiglas (a kind of Glass) with various thicknesses were simulated between 260 and 400 GHz (VNA measurement THz band) and the Crosslinked SUEX with various thicknesses were simulated between 100 and 2000 GHz (TDS measurement THz band). As shown in Fig. 2, the S_{21} of the PMMA is presented as an example to show that the S21 can be analyzed by the methods in Sect. 2.

As shown in Table 2, we estimated the ε'_r of these materials by using Eqs. (5) and (7). The estimated values approximate to the true values. It is found that the equations may not be applicable simultaneously in some cases. For example, the ε'_r of the 8 mm PMMA needs to be estimated by Eq. (5) as the peaks are not obvious for the $|S_{21}|$ of the PMMA, and the ε'_r of the 2 mm PVC needs to be estimated by Eq. (5) as the thickness of the PVC is less than a wavelength. Thus, the two proposed methods for ε'_r estimation should be used simultaneously. After estimation, the estimated ε'_r is adopted as the initial-value for the Newtons method. The tolerance of the algorithm is set to be 10e–7 according to Zhang et al. (2017). For each frequency, it takes about 0.14 second to converge using the initial value estimated by the proposed.

The extracted values of the Teflon, PVC, glass and crosslinked SUEX agree well with the true values as shown in Figs. 3 and 4. That further validates the proposed methods.

3.2 The dispersive sample in the literature

Those samples in the Part A have minimal variation in ε_r from low to high frequencies. To further show the excellent performance of the proposed, a dispersive sample



Fig. 2 S_{21} of three PMMA samples with different thickness

Material	Thickness (mm)	Frequency (GHz)	Method 1 (F-P resonance)		Method $2(\angle S_{21} = 180^{\circ})$	
			$\Delta f_1 (\mathrm{GHz})$	Estimated value	$\overline{\Delta f_2 (\mathrm{GHz})}$	Estimated value
РММА	4	260-400	23.04	2.6491	46.4	2.6127
	8		-	_	23.2	2.6127
	12		-	_	15.46	2.6141
Glass	2		29.45	6.4812	59.45	6.3661
	4		-	_	29.67	6.3898
	6		-	-	19.8	6.3769
PVC	2		45.75	2.6874	-	_
	4		29.12	2.9267	44.85	2.7964
	8		-	-	22.38	2.8076
Teflon	2		51.7	2.1045	-	-
	8		12.93	2.1028	25.88	2.0996
	16		6.47	2.0995	12.93	2.1028
Crosslinked	0.15	100-2000	617.5	2.6226	1247	2.5723
SUEX	0.45		205.25	2.6375	410.75	2.6342
	1		-	-	185.89	2.6046

Table 2 Estimated initial values (ε'_r) for the iterative algorithm



Fig. 3 Extracted complex permittivity of 16 mm Teflon, 8 mm PVC and 6 mm glass samples

Benzocyclobutene (BCB) with thickness of 2 mm is used for validation. The ε'_r is obtained from Seiler and Plettemeier (2019). The permittivity of the BCB is about 5.5 at 0.5 GHz, and is about 2.6 in the THz band as shown in Fig. 5. The permittivity of the BCB at low frequency is twice than that at the terahertz frequency.

As shown in Fig. 6, the extracted ε'_r of the BCB is wrong when using the permittivity at 4, 4.5 and 5 GHz as the initial values which are far away from the true values. And the values of the ε'_r extracted by the proposed method agree well with the true values.



Fig. 6 Extracted complex permittivity of 2 mm BCB with different initial values from 220 to 330 GHz

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4 Conclusions

In this work, a technique is proposed to estimate the permittivity of the MUT from the measured S_{21} . The estimated permittivity is a correct initial-value for the iterative technique which extracts the ε_r from the S_{21} . Since only the S_{21} can be efficiently measured in the THz band, the proposed is important for material characterization at THz frequencies. The proposed technique is efficient when the measured $|S_{21}|$ have peak values at multiple frequencies or the measured values of the $\angle S_{21}$ are equal to 180° at multiple frequencies.

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