Material Characterization in Partially Filled Waveguides Using Inverse Scattering and Multiple Sample Orientations

Daniel Sjöberg #1, Christer Larsson #*2

Electrical and Information Technology, Lund University
P.O. Box 118, S-221 00 Lund, Sweden
1 daniel.sjoberg@eit.lth.se
2 christer.larsson@eit.lth.se

* Saab Dynamics AB
S-581 88 Linköping, Sweden

***Abstract*—We present a method aimed at reducing uncertainties and instabilities when characterizing materials in waveguide setups. The S-parameters for a rectangular waveguide loaded with a rectangular sample block are measured for three different sample orientations, and the corresponding geometries are modeled in a finite element program, taking any material parameters as input. The material parameters of the sample are found by minimizing the squared distance between measured and calculated S-parameters.**

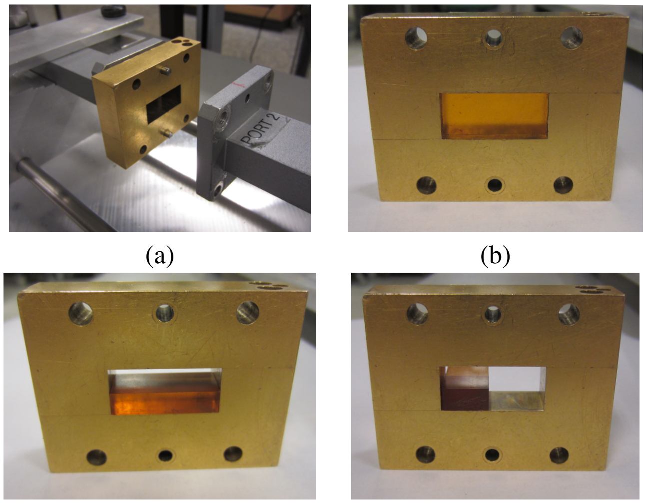
I. Introduction

The electromagnetic properties of materials are often characterized in a waveguide setup, where reflection and transmission data are used to compute permittivity and permeability of the sample, typically using the Nicolson-Ross-Weir (NRW) algorithm [1, 2]. However, this setup suffers from some important limitations: the sample needs to fit the cross section of the waveguide tightly, and when the length of the sample is close to one half wavelength, the NRW algorithm becomes unstable [3]. In [4, 5], it was shown that the latter of these problems is not due to the NRW algorithm itself, but rather the poor information in the reflection data, which becomes zero at the half wavelength frequency. In this paper, we investigate how more measurement data can be extracted from one single material sample, so that this loss of information can be counteracted.

II. Methods and Theory

Three different orientations of one single material sample were measured using the X-band setup described in [4, 5], see Fig. 1. The width of the waveguide is 22.9 mm, the height is 10.2 mm, and the length of the sample holder is 12.8 mm. By using TRL calibration [6], the measured S-parameters have reference planes at the edges of the sample holder.

The corresponding geometries were simulated with the commercial finite element program Comsol Multiphysics (www.comsol.com) using guessed complex material parameters $\epsilon_{\rm r} = \epsilon'_{\rm r} - {\rm j}\epsilon''_{\rm r}$ and $\mu_{\rm r} = \mu'_{\rm r} - {\rm j}\mu''_{\rm r}$. Waveguide ports were



(a) (b) (c) (d)

Fig. 1. (a) Sample holder attached to waveguide ports. (b) Sample filling the cross section of the sample holder (filled position). (c) Sample filling the width of the sample holder but not the height (side position). (d) Sample with its long dimension along the waveguide axis and flush against the left wall and bottom (end position).

defined at a distance of 5 cm from the position corresponding to the sample holder, and the resulting S-parameters were transferred to the sample holder edges by calibration.

When no model is assumed about the material behavior (apart from being homogeneous and isotropic), we need to determine the four real parameters $(\epsilon', \epsilon''_{\rm r}, \mu'_{\rm r}, \mu''_{\rm r})$ for each frequency of interest. This can be achieved by minimizing the penalty function

$$f(\epsilon_{\rm r}, \mu_{\rm r}) = \sum_{n=1}^{N}\sum_{i=1}^{2}\sum_{j=1}^{2} |S^{(n)}_{ij,\rm synt}(\epsilon_{\rm r}, \mu_{\rm r}) - S^{(n)}_{ij,\rm meas}|^2 \qquad (1)$$

where N is the number of sample positions, $S^{(n)}_{ij,\rm synt}$ are the synthetic S-parameters calculated by FEM, and $S^{(n)}_{ij,\rm meas}$ are the measured S-parameters. Many other penalty functions are of course possible.

Using a parameterized model for the material, for instance $\epsilon_r(\omega) = \epsilon_1 + \sigma/(j\omega\epsilon_0)$ and $\mu_r = \mu_1$, we can test the S-parameters at M frequency points using the penalty function

$$g(\epsilon_1, \sigma, \mu_1) = \frac{1}{M}\sum_{m=1}^{M} f(\epsilon_r(\omega_m), \mu_r(\omega_m)) \qquad (2)$$

More advanced models would typically contain sums of Debye and Lorentz models [7]. This approach is suitable if *a priori* knowledge of the frequency behavior is available.

The optimization was performed using the optimization routine `fmin` in the SciPy optimization package (www.scipy.org), which uses a downhill simplex algorithm. The Comsol simulation was controlled by a batch simulation model, taking material parameters and geometry of the sample as inputs, and writing the resulting S-parameters to a file which was subsequently read by the optimization penalty function.

III. Results

Two material samples were considered, both being nonmagnetic ($\mu_r = 1$) and having permittivities around 2.9 with small imaginary part. Their height and width were equal to the height and width of the rectangular waveguide, respectively, and their lengths were 5.1 mm (thin sample) and 9.6 mm (thick sample).

The optimization procedure minimizing f in (1) was applied at 11 equally distributed frequency points from 8 GHz to 12 GHz. Each frequency point was treated independently of the others, making no assumption of continuity of the material parameters. The same start guess, $\epsilon_r = 3 - 0j$ and $\mu_r = 1 - 0j$, was used for all points. For the frequency 8 GHz it was also verified that the optimization converged to the same value for the start guess $\epsilon_r = 1 - 0j$ and $\mu_r = 1 - 0j$. The optimization typically converged after about 200 evaluations of the penalty function f, corresponding to solving about 600 FEM problems. A parameter based optimization, minimizing g in (2), was applied using $M = 21$ frequency points between 8 and 12 GHz, which converged after about 200 evaluations of the penalty function g. Comsol can handle a frequency sweep efficiently enough to make the parameter based optimization converge in roughly the same time as one fixed frequency optimization. Thus, a major part of the computational burden is due to the numerous restarts of the commercial solver.

A. Thin sample

The 5.1 mm sample is shown in Fig. 1, with resulting S-parameters and material parameters in Fig. 2. In the top part of Fig. 2, it is seen that the reflection parameters S_{11} and S_{22} are not exactly on top of each other, revealing that the sample is not exactly symmetric. It is also seen that the variation with frequency is more pronounced for the partially filled cases, as can be expected.

The resulting material parameters are shown in the bottom part of Fig. 2, and compared to the output of the NRW algorithm [1, 2] for the case where the sample fills the cross section of the waveguide. It is seen that the fixed

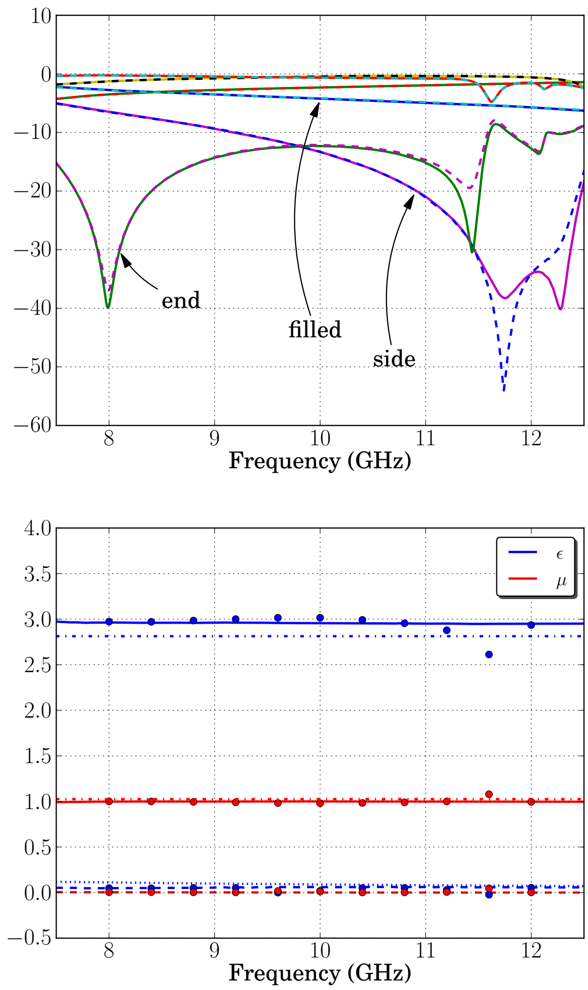


Fig. 2. Results for the 5.1 mm sample. Top: S-parameters in dB-scale for the three different sample orientations. The transmission parameters S_{21} and S_{12} are close to 0 dB, whereas the reflection parameters S_{11} and S_{22} are indicated by arrows. Bottom: Material parameters computed using the NRW method (solid lines), pointwise frequency optimization (dots), and parameter based optimization (dash-dotted lines). The real parts are close to 3 for the permittivity and close to 1 for the permeability, whereas the imaginary parts are close to 0 in both cases.

frequency optimization is performing well except at 11.6 GHz. Comparing with the behavior of the reflection parameters at the corresponding frequency, it is seen that they have sharp variations and probably do not present a well-defined minimum for the penalty function f. Excluding the reflection parameters for the “end” case from the penalty function at this frequency, we obtain $\epsilon_r(11.6\,\text{GHz}) = 2.64 - 0.045j$ and $\mu_r(11.6\,\text{GHz}) = 1.06 - 0.0015j$. These values are closer to the expected values, but are still not very accurate.

The parameter based optimization provides a permittivity significantly lower than the other methods. This may be due to the problematic reflection data at frequencies above 11 GHz just described, which can affect the whole frequency band since we are using a parameter based model for $\epsilon_r(\omega) = \epsilon_1 +$

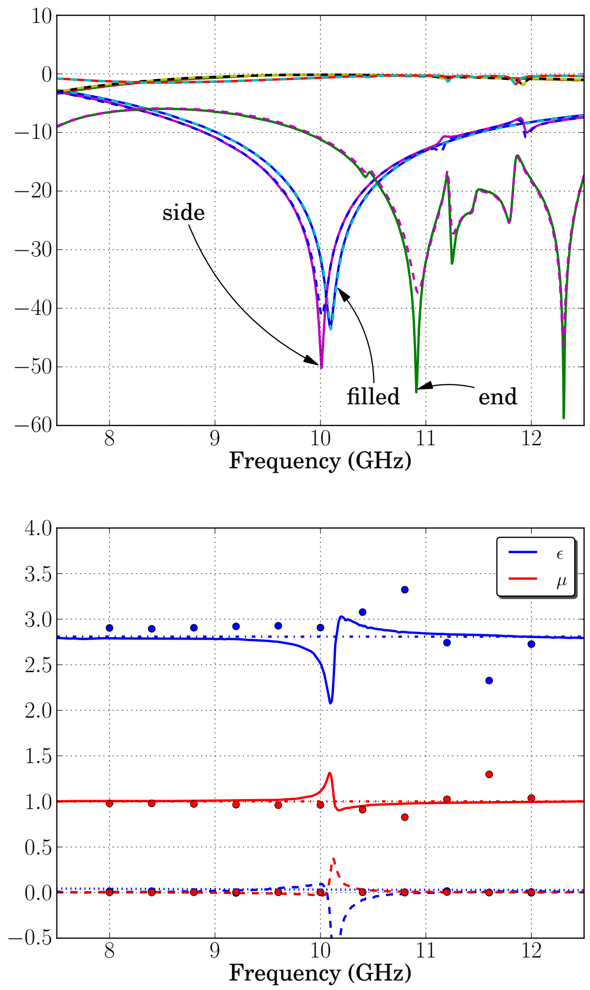


Fig. 3. Results for the 9.6 mm sample, organized as in Fig. 2. Top: S-parameters for the three different sample orientations. Bottom: Material parameters computed using the NRW method (solid lines), pointwise frequency optimization (dots), and parameter based optimization (dash-dotted lines).

$\sigma/(\mathrm{j}\omega\epsilon_0)$ and $\mu_\mathrm{r}(\omega) = \mu_1$. The explicit results are $\epsilon_1 = 2.81$, $\sigma = 0.049\,\mathrm{S/m}$, and $\mu_1 = 1.03$.

B. Thick sample

The thick sample is almost as thick as its height (9.6 mm compared to 10.2 mm. This makes the "side" position (corresponding to Fig. 1c) a situation with an almost filled waveguide, having a small gap. The sample is also thick enough to correspond to about half a wavelength at 10 GHz both in the "filled" and in the "side" position. This causes problems for the NRW algorithm at this frequency, as can be seen in Fig. 3. It is shown in [4, 5] that this is primarily due to the lack of information, since the reflection coefficient becomes very small at this frequency.

Having added more measurements, we see that the optimization approach is capable of accurately computing the complex permittivity and permeability, respectively, at this frequency. However, the optimization runs into some trouble of its own at even higher frequencies, particularly at 10.8 GHz and 11.6 GHz. Comparing with the S-parameters in the top part of Fig. 3, this behavior may be due to the strong frequency variation in the "end" case, possibly causing a less well defined minimum of f than at other frequencies. Recomputing these frequency points when excluding the reflection data for the "end" case from the optimization provides $\epsilon_\mathrm{r}(10.8\,\mathrm{GHz}) = 3.08 - 0.0084\mathrm{j}$, $\mu_\mathrm{r}(10.8\,\mathrm{GHz}) = 0.898 - 0.0082\mathrm{j}$, $\epsilon_\mathrm{r}(11.6\,\mathrm{GHz}) = 2.65 - 0.0050\mathrm{j}$, and $\mu_\mathrm{r}(11.6\,\mathrm{GHz}) = 1.05 - 0.0048\mathrm{j}$. These values correspond better to the expected values, but are still not very accurate.

The parameter based optimization seems to work better for the thick sample than for the thin, at least when comparing with the values given by the NRW algorithm. The explicit results are $\epsilon_1 = 2.81$, $\sigma = 0.018\,\mathrm{S/m}$, and $\mu_1 = 1.00$.

IV. Discussion

Even though the optimization is straight-forward, the use of a commercial FEM solver with limited control of the internal settings slows down the computations, so that the time to complete a single frequency point optimization in this first implementation is in the order of 10 hours on a desktop computer. With increased control of the solver, the gradient of the penalty function can be computed from the solution of the forward problem [8], and a gradient based optimization routine can be used with very little extra computational cost. This should reduce the number of evaluations of the penalty function f, which is particularly useful for problems with many parameters. Further, different penalty functions may help reducing the problems of the present implementation at higher frequencies.

V. Conclusions

We have demonstrated how redundant information from one material sample can be obtained by measuring reflection and transmission parameters in a waveguide setting for different orientations of the sample. Using all scattering parameters in an optimization approach to inverse scattering, fixed frequency real and imaginary parts of the permittivity and permeability could be determined. This was illustrated using real measurement data, and it is seen that the algorithm avoids the instability of the NRW algorithm at half wavelength resonance of the sample, but experiences some problems of its own at higher frequencies. These problems are probably due to the strong frequency variation of some of the scattering parameters. For samples known to have little or no frequency dependence, this can be handled by optimizing for parameters in a frequency dependent model of the material, typically a sum of Lorentz- and Debye-models.

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REFERENCES

[1] A. M. Nicolson and G. F. Ross, "Measurement of the intrinsic properties of materials by time-domain techniques," *IEEE Trans. Instrumentation and Measurement*, vol. 19, pp. 377–382, 1970.

[2] W. B. Weir, "Automatic measurement of complex dielectric constant and permeability at microwave frequencies," *Proc. IEEE*, vol. 62, pp. 33–36, 1974.

[3] J. Baker-Jarvis, E. J. Vanzura, and W. A. Kissick, "Improved technique for determining complex permittivity with the transmission/reflection method," *IEEE Trans. Microwave Theory Tech.*, vol. 38, no. 8, pp. 1096–1103, Aug. 1990.

[4] D. Sjöberg and C. Larsson, "Cramér-Rao bounds for determination of permittivity and permeability in slabs," *IEEE Transactions on Microwave Theory and Techniques*, vol. 59, no. 11, pp. 2970–2977, 2011. [Online]. Available: http://dx.doi.org/10.1109/TMTT.2011.2166085

[5] ——, "Opportunities and challenges in the characterization of composite materials in waveguides," *Radio Science*, vol. 46, pp. RS0E19–, 2011. [Online]. Available: http://dx.doi.org/10.1029/2011RS004644

[6] G. F. Engen and C. A. Hoer, ""Thru-Reflect-Line": An improved technique for calibrating the dual six-port automatic network analyzer," *IEEE Trans. Microwave Theory Tech.*, vol. 27, pp. 987–993, 1979.

[7] J. Baker-Jarvis, R. G. Geyer, and P. D. Domich, "A nonlinear least-squares solution with causality constraints applied to transmission line permittivity and permeability determination," *IEEE Trans. Instrumentation and Measurement*, vol. 41, no. 5, pp. 646–652, 1992.

[8] H. Akel and J. P. Webb, "Design sensitivities for scattering-matrix calculation with tetrahedral edge elements," *IEEE Transactions on Magnetics*, vol. 36, no. 4, pp. 1043–1046, jul 2000.