Dielectric Material Measurements Supported by Electromagnetic Field Solvers

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Abstract

An iterative transmission line technique for the determination of complex permittivity of non-magnetic, isotropic materials is addressed. The method is based on minimizing the objective function measuring the error between simulated and measured scattering parameters by classical Newton's method. An Electromagnetic field solver is used to solve the forward problem which is repeated in the application of Newton's method at each iteration. Since full-wave simulation is carried out, the method has no strict limitations on the geometry of the samples. For validation, proposed method is tested against partially loaded waveguide measurements at K-band.

1 Introduction

Determination of constitutive parameters of dielectric materials has a crucial importance in a wide range of practical applications of microwave theory. In the literature, there are many different techniques for material characterization such as transmission line methods [1], open-ended probes [2], resonator methods [3], and free-space methods [4]. Each technique has its own advantages and drawbacks when compared to the other ones. For instance, while transmission line technique leads to accurate results for broadband measurement, precisely machining of the specimen may be difficult, especially for higher frequencies. On the other hand, machining of the specimen is easier for open-ended waveguides, but accuracy of this method is lower than of the transmission line. Given measured data, in general, all techniques use the analytical but non-linear relation defined by its measurement configuration between material properties and scattering parameters to obtain material properties instead of full-wave modelling. Definitely, solving simple expression instead of full-wave simulation is time saving and straightforward when the analytical relation is able to model the measurement setup accurately. Deviation between the theoretical model and measurement setup can decrease the accuracy of the technique. Furthermore, it might be impractical to use standard techniques for some cases. For instance, in the case the material under test does not fill the whole cross section of the waveguide or has an arbitrary geometry, classical transmission line technique cannot be applied because there is no simple analytical expression for these cases. Therefore, full-wave simulation of the problem must be used to handle the problem. On the other hand, 3-D EM simulators have been widely used to analyse complex high-frequency problems during the recent years.

Within this context, the main aim of this study is to determine constitutive parameters of non-magnetic, isotropic materials for which classical techniques cannot be applied directly or lead to poor accuracy due to deviation of the measurement setup from the theoretical model. To this aim, an objective function is introduced as a measure for the error between measured and simulated scattering parameters. Starting from an initial guess, Newton's method is applied to find material properties by minimizing the objective function. Since scattering parameters and the Jacobian of the objective function have to be calculated at each iteration, a 3-D EM simulator (CST Microwave Studio) is used to solve the forward problem. This iteration scheme is continued until a predefined termination criteria is satisfied. In order to show validation of the method, measurements are performed at K-band for three different partially loaded waveguide configurations.

The most important advantage of the proposed method in contrast to classical material characterization methods is that it has no strict limitation on the geometry of the material to be tested. As a price for this advantage, the main drawback of the method is computational cost which is higher than for the classical techniques.

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2 Algorithm

The measured and simulated S-parameters are

$$\boldsymbol{S}^{\mathrm{m}} = \begin{pmatrix} s_{11}^{\mathrm{m}} & s_{12}^{\mathrm{m}} \\ s_{21}^{\mathrm{m}} & s_{22}^{\mathrm{m}} \end{pmatrix} = [s_{ij}^{\mathrm{m}}] \qquad \boldsymbol{S}^{\mathrm{s}} = \begin{pmatrix} s_{11}^{\mathrm{s}} & s_{12}^{\mathrm{s}} \\ s_{21}^{\mathrm{s}} & s_{22}^{\mathrm{s}} \end{pmatrix} = [s_{ij}^{\mathrm{s}}] \tag{1}$$

respectively. They depend on the relative permittivity $\varepsilon_{\mathrm{r}} = \varepsilon_{\mathrm{r}}' - \mathrm{j}\varepsilon_{\mathrm{r}}''$ and therefore

$$\boldsymbol{X} = \begin{pmatrix} \varepsilon_{\mathrm{r}}' \\ -\varepsilon_{\mathrm{r}}'' \end{pmatrix} = \begin{pmatrix} \mathrm{Re}\{\varepsilon_{\mathrm{r}}\} \\ \mathrm{Im}\{\varepsilon_{\mathrm{r}}\} \end{pmatrix} \tag{2}$$

is the parameter vector to be estimated from $\boldsymbol{S}^{\mathrm{m}}$. The quality of the estimate is measured by an objective function introduced as

$$\boldsymbol{F}(\boldsymbol{X}) = \sum_{ij} \begin{pmatrix} \beta_{ij}\,\mathrm{Re}\{s_{ij}^{\mathrm{m}} - s_{ij}^{\mathrm{s}}\} \\ \beta_{ij}\,\mathrm{Im}\{s_{ij}^{\mathrm{m}} - s_{ij}^{\mathrm{s}}\} \end{pmatrix} \qquad ; \qquad i,j = 1,2 \tag{3}$$

where β_{ij} is a weighting parameter between reflected and transmitted parameters and is chosen as $\beta_{11} = \beta_{22} = |s_{11}^{\mathrm{m}}|^2/|s_{21}^{\mathrm{m}}|^2$ and $\beta_{12} = \beta_{21} = 1$ to eliminate unstable solutions when the amplitude of reflection coefficient gets close to zero [1]. In fact, the expression in (3) is a modification of equation (24) in [1] by just replacing the explicit expression of scattering parameters with simulated ones. In the nth iteration step, the next (improved) guess is obtained by Newton's method through

$$\boldsymbol{X}_{n+1} = \boldsymbol{X}_n + [\boldsymbol{J}(\boldsymbol{X}_n)]^{-1}\boldsymbol{F}(\boldsymbol{X}_n) \tag{4}$$

where $\boldsymbol{J}$ is the Jacobian of the objective function and $\Delta\boldsymbol{X}_n = [\boldsymbol{J}(\boldsymbol{X}_n)]^{-1}\boldsymbol{F}(\boldsymbol{X}_n)$ is the step between subsequent iterations. To start the iteration an initial guess $\boldsymbol{X}_0$ is to be made. From numerical experiments, it is observed that $\boldsymbol{F}(\boldsymbol{X})$ is a holomorphic function. Hence, only derivatives with respect to the real part of the material properties in $\boldsymbol{J}$ are calculated by simply following three-point finite difference formula. The above iteration is terminated when $|\Delta\boldsymbol{X}|/|\boldsymbol{X}_n|$ becomes smaller than a predefined real number or a predefined iteration number is reached. Since there is no a priori information to choose a reasonable initial value for the first frequency, to avoid divergent results in the application of Newton's method, update amount is modified as

$$\Delta\boldsymbol{X} = \begin{pmatrix} \sqrt[n^2]{|s_{11}^{\mathrm{m}}|^2 + |s_{21}^{\mathrm{m}}|^2} & 0 \\ 0 & \sqrt[n^2]{1 - |s_{11}^{\mathrm{m}}|^2 - |s_{21}^{\mathrm{m}}|^2} \end{pmatrix} [\boldsymbol{J}(\boldsymbol{X}_n)]^{-1}\boldsymbol{F}(\boldsymbol{X}_n). \tag{5}$$

However, this modification which is only used for the first frequency calculations decreases the convergence rate but it makes the method more stable. Also, negative values of the imaginary part of the permittivity are forced to zero to avoid non-physical values. Then the result of the preceding frequency is used as initial guess for the next frequency.

3 Results

A rectangular waveguide with inner dimensions $x = 10.67\,\mathrm{mm}$ and $y = 4.32\,\mathrm{mm}$ was partially loaded with three different materials and the measurements were performed in the frequency range from 21 GHz to 24 GHz by a Vector Network Analyzer after Thru-Reflect-Line (TRL) calibration had been applied. For the first frequency calculation of all materials, initial guess is chosen as $\boldsymbol{X}_0 = (1 \quad 0)^T$ which corresponds to vacuum. Iterations were terminated when $|\Delta\boldsymbol{X}|/|\boldsymbol{X}_n|$ becomes smaller than 10^{-3} or iteration number reached $n = 16$. Rubber, Teflon and FR4 materials which have a rectangular prismatic shape with dimension $3.78\,\mathrm{mm} \times 4.32\,\mathrm{mm} \times 10.67\,\mathrm{mm}$, circular cylinder geometry with radius $r = 5.335\,\mathrm{mm}$ and height $h = 4.32\,\mathrm{mm}$, and a right-angled triangular prismatic shape with base $b = 10.67\,\mathrm{mm}$ and height $h = 4.32\,\mathrm{mm}$, respectively, were tested. Firstly, partially loaded waveguides were modelled and saved in CST Microwave Studio. Then, inversion algorithm was carried out by a MATLAB program which started full-wave simulation in CST Microwave Studio and retrieved the simulated scattering parameters for $\boldsymbol{X}_n$ and $\boldsymbol{X}_n \pm \triangle$ which are needed to calculate $\boldsymbol{F}(\boldsymbol{X}_n)$ and the three point estimation of $\boldsymbol{J}(\boldsymbol{X}_n)$, respectively. Inversion algorithm took per frequency 3.2 min, 2.9 min, and 5.1 min for rubber, Teflon and FR4, respectively. While there was discontinuity in x direction for rubber and Teflon, there was discontinuity in both x and y dimensions for FR4. Therefore, higher order modes exist for all configurations [5]. In order to compare the results, all materials were reshaped, then the well-known transmission line technique proposed by Baker-Jarvis *et al.* [1] was applied. The real and imaginary parts of the permittivity obtained by the proposed method are plotted in Figs. 1-3 together with Baker-Jarvis *et al.* [1] results for comparison. From the results, it can be concluded that the proposed method is quite capable of accurately characterizing materials having arbitrary geometry for which there may not even exist an analytical solution. By considering the initial guess $\boldsymbol{X}_0 = (1 \quad 0)^T$, the Fig. 3 shows that the sensitivity of method to initial value is poor. This is achieved by modifying update amounts as in equation (5).

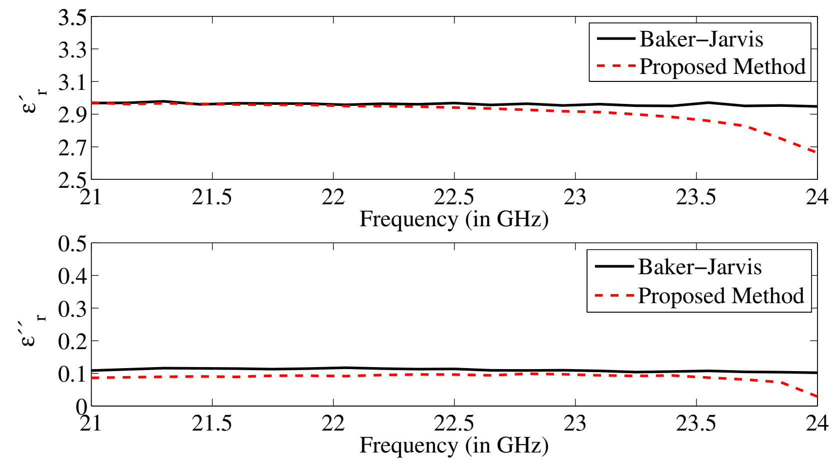

Figure 1: Estimated real and imaginary part of the permittivity of rubber.

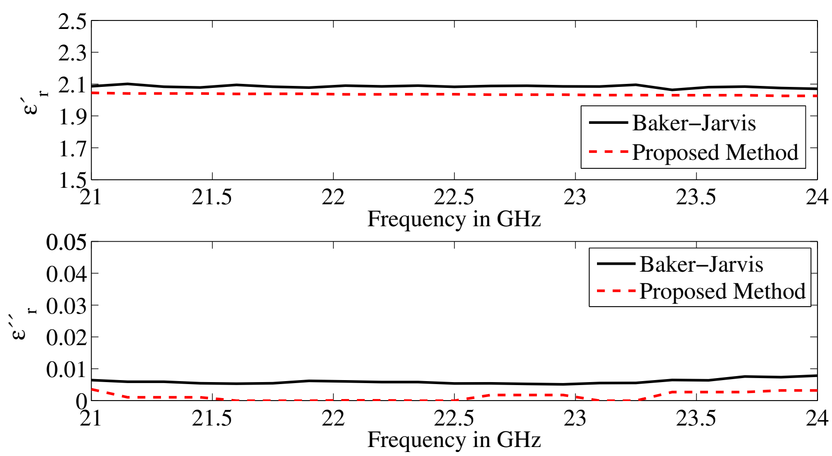

Figure 2: Estimated real and imaginary part of the permittivity of Teflon.

4 Conclusion

In this study, an iterative transmission line technique based on Newton algorithm for characterization of non-magnetic, isotropic material is presented. The method makes use of EM field solvers to perform full-wave simulation of the experimental setup. The Jacobian matrix of the objective function is calculated numerically

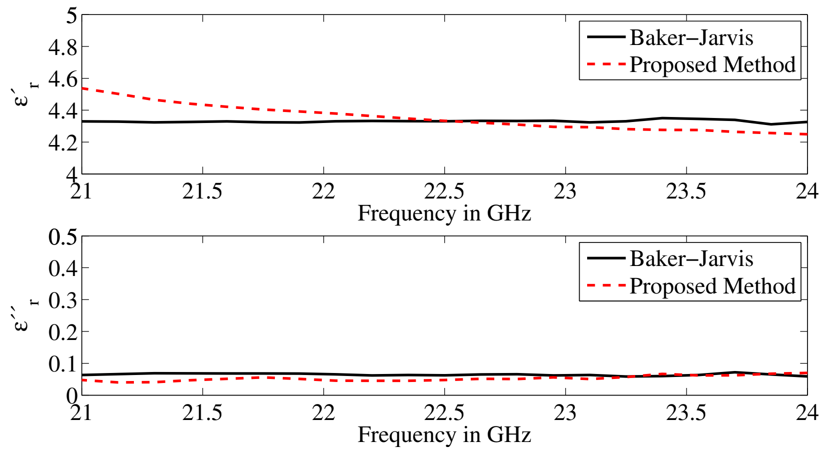

Figure 3: Estimated real and imaginary part of the permittivity of FR4.

by repeatedly solving the forward problem with EM field solvers at the neighbourhood points of the value for which derivatives are needed. The method is tested against partially loaded waveguide measurements and it is shown that the method is quite effective for measuring dielectric materials having almost arbitrary geometry. On the other hand, main drawback of the technique is computational time when it is compared to classical techniques. Since a 3-D EM simulator is used to model the characterization problem, the method can in principal be modified and applied to other material characterization techniques. Furthermore, the technique can be generalized for more complex problems having magnetic or anisotropic materials by applying higher order optimization technique i.e., quasi-Newton. Further studies will be developed in this direction.

5 References

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