Estimation of Material Permittivity in Free Space by Means of Inverse Problem Techniques

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Doctoral Thesis Summary

Tomas Bata University in Zlín

Tomas Bata University in Zlín
Faculty of Applied Informatics

Dissertation Thesis Statement

Estimation of Material Permittivity in Free Space by Means of Inverse Problem Techniques

Řešení inverzního problému odhadu permitivity materiálu ve volném prostoru

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ABSTRACT

The aim of the doctoral thesis is to design and implement a system for solving the inverse problem of estimation of electric permittivity of an unknown material or multiple layers of unknown materials. The proposed solution is based on the combination of an evolutionary algorithm and a direct mathematical model computing transmission and reflection coefficients of a defined material or a multi-layered structure of defined materials. Synthetic data as well as real data obtained by direct measurement of transmission and reflection coefficients in free space (frequency range: single units of gigahertz and higher) serve as the system input. Uncertainty and sensitivity analyses are also part of the study. Included experiments present reasonable estimations of complex permittivity with rather low uncertainties and low sensitivity on the error of the input data.

ABSTRAKT

Doktorská práce je zaměřena na návrh a implementaci systému řešícího inverzní problém určení elektrické permitivity neznámého materiálu či vrstev neznámých druhů materiálu. V navrženém řešení je využita kombinace evolučního algoritmu a přímého matematického modelu vypočítávajícího koeficienty odrazu a prostupu definovaného materiálu či vícevrstvé struktury definovaných materiálů. Vstupem systému jsou přitom právě koeficienty odrazu a prostupu ve volném prostoru ve frekvenčním rozsahu od jednotek gigahertz výše. V práci je též věnován prostor citlivostní analýze i analýze nejistot implementovaného sytému. Součástí práce jsou i experimenty jak se syntetickými daty, tak i s daty z přímých měření prokazující použitelnost navrženého systému. Odhady komplexní permitivity provedené v rámci experimentální části jsou uspokojivé, s poměrně nízkou mírou nejistot a současně s přijatelnou tolerancí vůči úrovni chyby u vstupních dat.

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1 INTRODUCTION

The importance of material properties awareness is rising. In the last few decades, new artificial materials have been developed, but in most cases, their properties have not yet been fully described. This lack of knowledge and the need to enable people to work with these new types of materials give scientists the opportunity to bridge this significant gap.

The aim of this work was to find a solution – or rather one of possible ways – to estimate electromagnetic properties of an unknown material or several unknown materials in a layered structure.

The doctoral thesis describes the process of design of a new system estimating complex permittivity of a single or multi-layered structures of non-magnetic homogeneous isotropic materials of known thicknesses. The aim of this work is also to develop a software tool implementing the theoretical system in order to help scientists and material engineers to estimate properties of unknown materials. The number of such materials has grown in the last decade. This is mainly due to numerous modern nanomaterials, polymers and composites. These materials are usually produced with limited information related to their properties, such as complex permittivity (moreover, in higher frequencies corresponding to sub-millimeter waves).

The project presented in this thesis is based on synthetic as well as measured transmission coefficients. Measurements in free space have been selected so as to enable measuring transmission coefficients even in very high frequencies (up to single units and tens of terahertz). The measured parameters are processed in a system for backward reconstruction of permittivity employing an evolutionary algorithm. This process is described in more detail below.

The presented system for backward reconstruction of complex permittivity has been tested using synthetic data as well as using noisy synthetic data and real (measured) data. The results of these experiments, including uncertainties, are also part of the thesis.

2 STATE OF THE ART

Basic theoretical fundamentals of this work including the relation among the complex permittivity of a material, its thickness and the transmission/reflection coefficients is mentioned in this section.

2.1 Complex Electric Permittivity

Electric permittivity is a constant of proportionality (in a closed frequency range) that exists between electric displacement field D and electric field intensity E (in free space):

$$\epsilon = \frac{D}{E} \tag{2.1}$$

Permittivity divided by permittivity of vacuum (a constant, $\epsilon_0 = 8.8542\ pF/m$ approx. [11]) is called relative permittivity (relative to the vacuum):

$$\epsilon_r = \frac{\epsilon}{\epsilon_0} \tag{2.2}$$

Relative permittivity of an isotropic dielectric is a scalar constant considering usual (low) frequency ranges. This assumption may not be true when considering wide ranges or ranges of higher frequencies. Permittivity as a quantity used to describe dielectric properties that influence reflection of electromagnetic waves at interfaces and the attenuation of wave energy within materials [14]. The complex relative permittivity ϵ_r^* of a material can be expressed in the following form [10]:

$$\epsilon_r^* = \epsilon_r' - j\epsilon_r'' \tag{2.3}$$

$$j = \sqrt{-1} \tag{2.4}$$

The real part ϵ_r' is referred to as the dielectric constant and represents stored energy when the material is exposed to an electric field, while the dielectric loss factor ϵ_r'', which is the imaginary part, influences energy absorption and attenuation [14].

2.2 Computation of Transmission and Reflection Coefficients

Correct valid theory must be placed and implemented while thinking about using a direct model computing transmission/reflection coefficients. Therefore, some fundamental equations derived from Maxwell's theory are presented below to reveal the computational mechanism. Only perfect mathematical model can be joined with an evolutionary algorithm and thus assure acceptable estimations of complex permittivities of materials.

The list of the input data to the direct model follows (considering a multi-layered structure of materials under test):

- number of layers,
- relative permittivity of each layer,
- thickness of each layer,
- angle of incidence, and
- set of frequency points.

A possible multi-layered structure is depicted in Fig. 2.1. There are three sections of materials in this illustration. The first and the third layer is of the same material #1 with the same thickness (d_1). The incident plane waves come perpendicularly (the angle of incidence $\Theta = 0$). This sandwich structure may be also used to estimate properties of some liquid as material #2.

The contemporary literature is saturated with mathematical descriptions of propagation through materials of known properties. Fundamental theory and equations based on previous research [3, 10, 17, 13] with its further explanation follows:

$$\sigma = -\epsilon_r' \, \epsilon_0 \, \omega \, \tan(\delta) \tag{2.5}$$

$$Z_{m-1} = K_{m-1} \frac{Z_m + K_{m-1} \tanh(U_{m-1} d_{m-1})}{K_{m-1} + Z_m \tanh(U_{m-1} d_{m-1})} \tag{2.6}$$

$$\gamma_m^2 = -\mu_m \, \epsilon_{rm} \, \epsilon_0 \, \omega^2 + j \, \sigma_m \, \mu_{rm} \, \mu_0 \, \omega \tag{2.7}$$

$$L = j \, \gamma_0 \, \sin(\Theta) \tag{2.8}$$

$$U_m = \sqrt{L^2 + \gamma_m^2} \tag{2.9}$$

$$K_0 = \sqrt{\frac{\mu_0}{\epsilon_0}} \, \cos(\Theta) \tag{2.10}$$

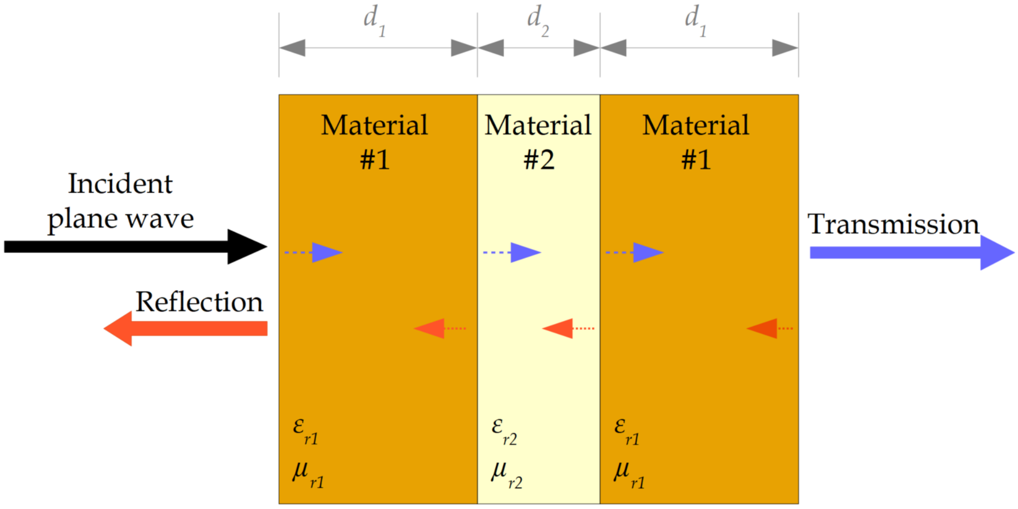

Fig. 2.1 Schema of a sandwich structure of materials under test, side view, incident plane waves come from the left, S_{11} represents the reflection and S_{21} is the transmission on the structure

$$K_m = \frac{U_m}{\sigma_m + j\ \omega\ \epsilon_{rm}\ \epsilon_0} \tag{2.11}$$

$$R_0 = \frac{K_0 - Z_1}{K_0 + Z_1} \tag{2.12}$$

R_0 represents the desired reflection coefficients on the layered media related to the specific frequency f (and corresponding angular frequency ω). Each layer of a material (subscript $_m$) is represented by complex relative permittivity $\epsilon'_{rm} - j\epsilon''_{rm}$, relative permeability μ_{rm}, thickness d_m, conductivity σ_m, loss tangent $\tan\delta_m$, wave impedance Z_m, wave impedance of the incidence region K_m (whereas Θ stands for the angle of incidence) and, finally, propagation constant U_m. The values of R_0 are absolute values (not logarithmic) of the closed interval of $[0.0, 1.0]$.

There is a free space before and after the layered structure under test (this thesis is aimed at free space measurements). Therefore, the wave impedance of the last layer is given by $Z_n = K_0$ (where n is equal to the number of layers).

2.3 Evolutionary Algorithms

Evolutionary algorithms (EAs) belong to the area of artificial intelligence. They are stochastic population-based metaheuristic algorithms. Such algorithms are used in single-objective (or more often) in multi-objective optimization problems (MOPs) [4]. Genetic Algorithm, Differential Evolution, Particle

Swarm Optimization and Self-Organizing Migrating Algorithm are common representatives of the EAs.

A problem to be solved in an EA has to be mathematically explicitly expressed. Such an expression is used in so called *fitness function*. This function is responsible for computing the fitness of all the individuals in each iteration of an EA. Consequently, the fitness value plays a significant role in the process of creating a new generation. This process vary throughout the group of EAs.

3 RESEARCH AIMS AND OBJECTIVES

Nowadays the boom of development of new artificial materials (like various kinds of composites, polymers and nanomaterials) is so great that developers, constructors, engineers, physicists, chemists and scientists in general can select from an enormous spectrum of materials and ways of how to compile their design, construction or product. The utilization could be much wider if there was information about all properties of such materials. This study is going to help to define one specific property: the complex permittivity.

This work is aimed at help in estimation of the permittivity of unknown non-magnetic homogeneous isotropic materials. Therefore, the most applicable general idea (i.e., the problem) is that there is an unknown material and there is a need to define it (or at least its properties). This is the direct application of the system developed in the doctoral thesis. The submission is wide and the doctoral thesis may be designated as multidisciplinary because of its relations with the areas of material science, mathematics, applied information technology and measurement.

The objectives of this thesis can be summarised into the following list:

- synthesis of a direct mathematical model computing reliable scattering parameters (S-parameters, containing transmission and reflection coefficients) of a single or multi-layered structure of defined materials in free space at certain frequency range based on literature review, where the materials are non-magnetic homogeneous isotropic,
- implementation of the direct model into a software,
- verification of the direct model by comparing its computed synthetic S-parameters with S-parameters obtained by direct measurements,

- implementation of an evolutionary algorithm (EA) into the software and combination with the direct model,
- experimental part: comparison of the permittivities of known standard materials with the permittivities estimated by the developed system using synthetic S-parameters as well as S-parameters obtained by direct measurements, and
- elaboration of the uncertainty and sensitivity analysis of the final system.

4 METHODOLOGY

This section contains an overview of the methods, main technologies and approaches used in this work.

4.1 Applied Scientific Methods

The list of scientific methods which have been employed in this work follows:

- analysis of the state of the art related to the electric permittivity, EAs and S-parameters,
- hypothesis about development of a new way of complex permittivity estimation based on backward reconstruction using measured S-parameters,
- synthesis of a direct mathematical model capable of computing reliable S-parameters of a given single material or a multi-layered structure,
- synthesis of the direct model and an EA into a software instrument using a programming technology,
- experiments with the software developed in the previous step using data synthesized by the direct model itself,
- comparisons of the output of the experiments from the previous step with the expected permittivities of the materials (and thus verifying the implementation of the combination of the direct model and the EA),
- experiments with real known materials, direct measurements of their S-parameters and estimating their permittivities using the developed software instrument,
- comparisons of the estimated permittivities of materials in the previous experiment with their expected permittivities,
- repetitions of the previous experiments with results comparisons and also

experimenting with different materials (various experimental setups),
- analysis of sensitivity of the software instrument on the input error level, and
- analysis of uncertainties of the output of the software instrument in various experimental setups.

4.2 Measurements in Free Space Employing VNAs

The interest of this work is situated in the area of microwaves what means the range from units to hundreds of GHz approximately with respect to the frequency. There is one insuperable reason for measuring in free space against the measurement using a waveguide. The reason relates to the frequency range of interest. It is planned to work with frequencies higher than units of GHz. Dimensions of a typical waveguide for such a task are too low. Common rectangular waveguides for V-Band: R620 (frequency band of operation: 50.00 GHz – 75.00 GHz; cutoff frequency of lowest order mode is at 39.875 GHz; cutoff frequency of the next mode is at 79.750 GHz) have inner dimensions 3.759 mm × 1.880 mm [7]. These dimensions are too low and become even lower with higher frequencies. Therefore, the limitations in dimensions does not allow to work with waveguides at the planned range of frequencies.

A material under test must be placed between the sending and receiving horn antennas. The information from the antennas (reflection and transmission coefficients, S_{11} and S_{21} respectively) is then captured by a calibrated vector network analyser (VNA).

4.3 Software for S-Parameters Post-Processing

The software post-processing the measured S-parameters has been written in C++ programming language (using current standard C++17). The reason for this choice is the efficiency and speed of the software written in this language, simple portability between different architectures and operating systems. C++ is a modern, object-oriented and also performance-oriented programming language. The final software runs in a command-line/terminal environment with possibility of running with parameters what represents a robust approach in the point of view of automatized sequential as well as parallel launching in a batch.

The problem solved in this thesis is a MOP. Each layer in multi-layered structures under test is represented by two unknowns, it is the real and the imaginary part of the complex relative permittivity.

This work is not aimed at analysis and comparison of multiple EAs presenting their capabilities or differences. This topic is covered by available literature (for instance [4]). Particle Swarm Optimization (PSO) has been selected for implementation into the developed system. This choice is also based on the author's previous research and experiences in the area of inverse processing. PSO is robust and fast enough. PSO does not require special configuration and enables setting of intervals for each design parameter. A framework called *Population based Optimization Toolbox* (POPOT) written in C++ is used as the working implementation of PSO. This framework has been published under GNU General Public Licence (GPL) version 3 [8] and thus it is legal to use it freely in this doctoral thesis.

The fitness function in PSO is performing evaluation of each particle. Such an evaluation is represented by computing the norm of the vector defined by position of given and computed complex S-parameters. This is generalized in the following formula:

$$\begin{aligned} f_p^2 = {} & (S_{g1\_real} - S_{c1\_real})^2 + (S_{g1\_imag} - S_{c1\_imag})^2 \\ & + (S_{g2\_real} - S_{c2\_real})^2 + (S_{g2\_imag} - S_{c2\_imag})^2 \\ & + \ \dots \\ & + (S_{gn\_real} - S_{cn\_real})^2 + (S_{gn\_imag} - S_{cn\_imag})^2 \end{aligned} \tag{4.1}$$

where f_p stands for the fitness of a particular particle p, S_{gi} is the given i-th S-parameter (from an input file containing measured or synthetic data), S_{ci} is the computed i-th S-parameter of the particle and n is the total number of S-parameters (the dimensionality of the vector). Usually there are only absolute values of the measured S-parameters at the input. Therefore, the difference between each measured and computed S-parameter ($S_{gn} - S_{cn}$) is set by the difference of the absolute values. Therefore, the fitness value is evaluated as:

$$f_p = \sqrt{(|S_{g1}| - |S_{c1}|)^2 + (|S_{g2}| - |S_{c2}|)^2 + \cdots + (|S_{gn}| - |S_{cn}|)^2} \tag{4.2}$$

Similar Root Mean Square (RMS) would be also applicable. But in this particular case the division before computation of the square root is an expensive mathematical operation from the point of view of the processing time of a central processing unit (CPU) and, moreover, it is not beneficial in this case due to the constant value in the denominator.

4.4 Adding Noise to the System Input

In the specific experiments and sensitivity analysis some noise had to be added to the system input to verify the system robustness and also to perform the uncertainty and sensitivity analyses.

One of the key characteristics in SI measurements is jitter. It represents variations in the data signal. Typically, these variations behave statistically in nature. Random jitter usually follows a normal distribution [2]. Classical statistical methods that use the sample mean and standard deviation, under the assumption that the data follow a Gaussian (normal) distribution, are often applied to measurement inter-comparisons [12]. Therefore, the noise to be added to the input S-parameters should follow the normal distribution with specified standard deviation.

The noise is applied on the input S-parameters in the following way:

$$S'_g = S'_{in} R(\mu, \sigma) \tag{4.3}$$
$$S''_g = S''_{in} R(\mu, \sigma) \tag{4.4}$$

where S'_{in} and S''_{in} are the real and the imaginary parts of the complex input S-parameter, $R(\mu, \sigma)$ represents a pseudorandom numbers generator (PRNG) of normal distribution with mean $\mu = 1.0$ and standard deviation σ is the relative standard deviation (RSD, also known as the coefficient of variation). S'_g and S''_g represent the real and the imaginary parts of the given complex S-parameter used in the further processing in the algorithm.

RSD is used in order to provide better readability and possibly easier understanding in the rest of this work. RSD is equal to standard deviation σ divided by mean μ [16]:

$$c_v = \frac{\sigma}{\mu} \tag{4.5}$$

With respect to the mean $\mu = 1.0$ the value of RSD is equal to the value of standard deviation σ. This is the case of application of noise on the input S-parameters.

4.5 Simplifications

Introduced approach is quite complicated with respect to the nature of this inverse problem. The problem of estimation of permittivities of multi-layered structures from S-parameters seems not to be explicit. Therefore, the problem is not closed to just one solution, it is ambiguous, not deterministic and more solutions may be produced. Then there is also a space for some expert system limitations (like some reasonable expectable boundaries of relative permittivities). The more unknown variables to be estimated (more layers, more dimensional space has to be searched) the more complicated and longer processing along with a risk of possibly higher number of possible solutions. This problem becomes hard to solve for more than one unknown layer with respect to the real and the imaginary part of the complex permittivity. Therefore, in the simplified case when the thickness of each layer is known there are two unknowns per layer. For two layers there are four unknowns, six unknowns for three layers. That is why this is the right place for utilization of EAs.

Considering such a MOP the situation could be intentionally simplified in neglecting the fact that the permittivity could (and very probably does) depend on frequency. In this work the real part of the complex permittivity is wilfully considered as a constant (in a narrow frequency range). This is highly important to mention at this place. This shortage can be removed in the future after incorporation of this specific part into the whole system.

5 EXPERIMENTS

The designed system implemented into a software instrument has to be tested to verify its correctness. Therefore, several kinds of experiments have to be performed:

1. The software must be tested using synthetic data of single and multi-layered structures generated by the implemented direct mathematical model to verify the capability of the backward reconstruction using the selected EA.
2. The software must be tested using noisy synthetic data of single layers as well as on data of multi-layered structures to test the reasonable robustness of the backward reconstruction.

3. The software must be tested also using S-parameters obtained by direct measurements of single layers as well as of multi-layered structures of several materials to verify the inner direct mathematical model computing S-parameters and the whole system in general. This kind of tests represents the most difficult cases.

5.1 Materials Under Test

Several experiments have been done with aluminium oxide, FR-4, plexiglass and polytetrafluoroethylene (PTFE). These materials have been already successfully defined and standardized in the past. These dielectrics have clear material properties and ease of access. Therefore, they are suitable for experiments in this work. These materials are briefly described below.

The combinations of materials in multi-layered structures in the following experiments does not have a practical meaning (or it was not intended at least). They are just combined for testing purposes without any subsidiary intentions.

Basic relevant information about the materials under test:

- Aluminium oxide:
  - $\epsilon_r = 9.424$ (at 17 GHz; depends on the purity of the selected material, 99.6 % Alumina in this case); loss tangent: 0.00031 [18],
  - shape and dimensions of tested material: block, 50 mm x 50 mm x 10 mm.
- FR-4:
  - $\epsilon_r = 4.2 - j0.084$ (at 1 GHz); loss tangent: 0.02 [6],
  - shape and dimensions of tested material: sheet, 1.53mm thickness.
- Plexiglass:
  - $\epsilon_r = 2.5 - j0.02$ (at 10 GHz); loss tangent: 0.005 [21],
  - shape and dimensions of tested material: sheet, 3.66mm thickness.
- PTFE:
  - $\epsilon_r = 2.05 \pm 0.05 - j0.04$ (at 3 GHz); loss tangent: 0.00028 [20],
  - shape and dimensions of tested material: cylinder, 50mm diameter, 3.0mm thickness.

5.2 Setup of the Evolutionary Algorithm

The Particle Swarm Optimization has been experimentally set to use 60 individuals in a swarm. Number higher than 100 usually makes the process of reconstruction ineffectively longer, without achieving a better precision [4].

The EA is set up to stop if the fitness value (the square root of a sum of differences of computed and given S-parameters powered by two) is less than 10^{-7} or if the count of these evaluations is higher than 20 000 multiplied by the number of dimensions of solved problem (two dimensions for a single layer, four dimensions for a double layer etc.).

The lower and upper bound of a permittivity has been set up to the following intervals:

- $[1.0, 15.0]$ for the real part of the complex permittivity, and
- $[0.0, 1.0]$ for the imaginary part of the complex permittivity.

The upper bound has been set to the value of 15.0 which should represent a sufficient value for usually used solid dielectric materials (and with respect to the selection of materials under test in this work).

5.3 Test Computer

Subsequent experiments with the developed software have been run on a computer manufactured in 2016. It is Dell Latitude E5570 with processor Intel® Core™ i7-6820HQ 4x 2.7 GHz, 16 GB RAM, operating system: Microsoft Windows 10 Professional 64-bit.

The software is executable also in Linux operating systems. The processing times in Linux are similar to the processing times in Microsoft's Windows operating system. However, they are not presented in the thesis.

5.4 Experiment: Noisy Synthetic Data of a Multi-Layered Structure

In this scenario the robustness of the implemented backward reconstruction is tested on data from multiple layers including some additional noise.

Tab. 5.1 Results of the experiment with noisy synthetic data of a 3-layered structure consisting of PTFE & air & PTFE, noise of 5% RSD

Iteration	*Estimated* ϵ_{r1}	*Estimated* ϵ_{r2}	*Estimated* ϵ_{r3}	*Fitness (the best)*	*Time [ms]*
1	$2.072-j0.043$	$1.002-j0.000$	$2.020-j0.045$	0.544	14 536
2	$2.029-j0.045$	$1.000-j0.005$	$2.018-j0.015$	0.524	15 289
3	$2.113-j0.023$	$1.015-j0.000$	$2.028-j0.042$	0.542	14 781
4	$2.082-j0.049$	$1.011-j0.001$	$1.979-j0.054$	0.510	15 539
5	$2.062-j0.033$	$1.001-j0.001$	$2.044-j0.041$	0.497	15 855
6	$2.059-j0.051$	$1.000-j0.000$	$2.012-j0.058$	0.514	14 799
7	$2.097-j0.039$	$1.000-j0.006$	$1.976-j0.017$	0.479	15 648
8	$2.057-j0.041$	$1.000-j0.006$	$2.021-j0.033$	0.529	15 501
9	$2.019-j0.036$	$1.000-j0.000$	$2.091-j0.045$	0.447	14 419
10	$2.097-j0.034$	$1.003-j0.000$	$2.042-j0.034$	0.526	14 589
Average	$2.0686-j0.0395$	$1.0031-j0.0018$	$2.0231-j0.0384$	0.5112	15 095.6

The synthetic S-parameters of three layers of imaginary materials are used in this experiment. The structure consists of PTFE, air and PTFE again (some kind of a sandwich structure). The thicknesses of the sections are 3.0, 10.0 and 3.0 mm. S-parameters are synthesized at 201 frequency points, from 1.0 to 20.0 GHz. Moreover, some noise has been added to the generated S-parameters (normal distribution, RSD 5 %).

The system responded well. The average estimated complex relative permittivity of the first, the second and the third layer is:

1. $\epsilon^*_{r1} = 2.0686 - j0.0395$,
2. $\epsilon^*_{r2} = 1.0031 - j0.0018$, and
3. $\epsilon^*_{r3} = 2.0231 - j0.0384$.

These are the average values from 10 runs of the software, see Tab. 5.1. The relative deviations in this experiment are equal to 0.9 %, 0.3 % and 1.3 % (regarding the absolute values of the expected and the average estimated permittivities of the layers). The average estimated permittivities are very close to the original (expected) complex relative permittivities. This confirms some robustness of the backward reconstruction system.

5.5 Experiment: Measured Data of a Multi-Layered Structure

This measurement took place at the Department of Dielectrics at Institute of Physics of the Czech Academy of Sciences in Prague.

A 2-layered structure of Aluminum oxide and PTFE has been measured on 21 frequency points from 448 GHz to 737 GHz. The average estimated complex relative permittivity of the first material from the structure (Aluminum oxide) was $9.8642 - j0.00004$ and $1.8725 - j0.46995$ of the second material, the average processing time was 1 160.4 ms (average values from 10 runs of the software).

These results' relative deviations are equal to 4.7 % and 5.8 % for the first and for the second material respectively (regarding the absolute values of the expected and the average estimated relative permittivity). These results are acceptable. They confirm the capability of the developed system to work with data from direct measurements of multi-layered structures.

5.6 Summary of the Experiments

Realization of experiments posed a more complicated task than expected. Acquisition of materials was rather easy part in comparison with negotiations with laboratories postponing the measurements. This is the main reason why the number of materials under test and the corresponding number of direct measurements presented in the full version of the doctoral thesis is not high. However, the number of experiments can be considered as sufficient for the need of confirmation of the individual pillars, approaches and implementations.

The speed of the implemented system is noted in the tables and paragraphs in each free-space experiment. The processing time mainly depends on the number of layers in the experiment, afterwards, on the number of frequency points and also on the hardware on which the software is executed.

6 UNCERTAINTY & SENSITIVITY ANALYSIS

Quantification of the uncertainty of any measurement is important since there is always a margin of doubt about the measurement. The uncertainty of the estimation of permittivity in free space is not analytically solvable due to the fact that the problem of permittivity reconstruction is not an explicit problem. ϵ_r cannot be computed directly using a mathematical formula (see section 2). Therefore, the uncertainty is estimated statistically by a set of repetitions of permittivity estimations (so called Type A evaluation [1]).

The source of error in the estimation of permittivity is represented by a combination of the error in the measuring instrument (for instance: bias, changes due to ageing, wear, noise, wrong calibration), the deviations in the material under test (for instance: non-homogeneousness, impurities) and environment issues (for instance: higher or lower temperature or humidity). The combination of all these influences leads to a mass error of the input data (S-parameters). Therefore, an input error represented by a RSD is included in the analysis.

6.1 Pseudorandom Number Generator

The role of the pseudorandom number generator (PRNG) is important not only in the process of evolution in EAs but also in the experiments adding some noise to the input S-parameters. The noise must follow a desired probability distribution.

Standard random numbers generator available in C++ has been used in the developed software. The implementation of PRNG should follow to the desired normal distribution. However, this hypothesis should be verified. For this purpose, the Pearson's chi-square goodness of fit test [19] has been applied on the pseudorandomly generated data. This test is used to confirm or reject a null hypothesis. Working with observed data generated by selected PRNG, the null and the corresponding alternative hypotheses are the following:

- H_0: The observed data are normally distributed.
- H_A: The observed data are not normally distributed.

Configuration of the chi-square goodness of fit test:

- The PRNG has been set up to produce numbers following the standard normal distribution ($\mu = 0.0$, $\sigma = 1.0$).
- Histogram is portioned into $k = 20$ segments.
- The significance level in this test has been set to $\alpha = 0.05$ (common

threshold [5]).

- The sum of the empirically counted numbers and the sum of generated numbers is 99 992.

Results of the test: $n = 17$, $\chi^2 = 24.961$, $p = 0.929$.

Conclusion: H_0 is accepted on the significance level alpha ($p \leq 1 - \alpha$).

This test has been repeated and the hypothesis H_0 was accepted in 9 from 10 cases (10 test sets of pseudorandom numbers).

6.2 Experiment: a 3-Layered Structure

Only the most complicated case under uncertainty & sensitivity analysis is presented in this statement. It is a 3-layered structure (three pairs of real and imaginary parts of complex relative permittivities what means a six-dimensional optimization problem). The combination of PTFE, FR-4 and plexiglass has been tested in this experiment. The number of repetitions of all the tests in this analysis has been set to 100.

The input data (S-parameters) in these experiments must be strictly correct to evaluate proper total output uncertainty of the result and sensitivity analysis on the controlled artificial input error. These input data have been synthesized by the implemented direct model in the frequency range from 1 to 20 GHz. This rather narrower range has been selected so as to consider constant real part of complex permittivities of the materials under test, moreover, without complications caused by resonances.

The estimated complex relative permittivities with statistically defined standard uncertainties and analysis of sensitivity on error level of the input data using 201 frequency points is presented in Tab. 6.1. The mean values of the real and the imaginary parts of the complex relative permittivity including uncertainties are also depicted in Fig. 6.1.

Tab. 6.1 Estimated complex relative permittivity with statistically defined standard uncertainty along with sensitivity analysis on RSD of the error of the input data, a 3-layered structure, expected $\epsilon_{r_1} = 2.05 - j0.04$, $\epsilon_{r_2} = 4.2 - j0.084$ and $\epsilon_{r_3} = 2.5 - j0.02$, 201 frequency points

Noise RSD	$\overline{\epsilon_{r1\ real}} \pm u_{1\ real}$	$\overline{\epsilon_{r1\ imag}} \pm u_{1\ imag}$	$\overline{\epsilon_{r2\ real}} \pm u_{2\ real}$	$\overline{\epsilon_{r2\ imag}} \pm u_{2\ imag}$	$\overline{\epsilon_{r3\ real}} \pm u_{3\ real}$	$\overline{\epsilon_{r3\ imag}} \pm u_{3\ imag}$	$\bar{t}$ [s]
0 %	2.0450 ± 0.0013	0.040384 ± 0.000071	4.1921 ± 0.0020	0.0796 ± 0.0011	2.5084 ± 0.0022	0.02057 ± 0.00013	13.3
1 %	2.0441 ± 0.0090	0.0419 ± 0.0044	4.1824 ± 0.0035	0.0714 ± 0.0033	2.515 ± 0.010	0.01952 ± 0.00086	13.6
2 %	2.0586 ± 0.0095	0.0510 ± 0.0048	4.1800 ± 0.0051	0.0858 ± 0.0049	2.491 ± 0.012	0.0216 ± 0.0014	14.2
5 %	2.104 ± 0.015	0.0774 ± 0.0083	4.1803 ± 0.0099	0.1086 ± 0.0084	2.433 ± 0.019	0.0236 ± 0.0019	13.8
10 %	2.137 ± 0.012	0.116 ± 0.013	4.092 ± 0.022	0.163 ± 0.013	2.353 ± 0.022	0.0348 ± 0.0026	13.9
20 %	2.141 ± 0.017	0.195 ± 0.021	4.061 ± 0.036	0.190 ± 0.017	2.294 ± 0.031	0.0303 ± 0.0029	13.6

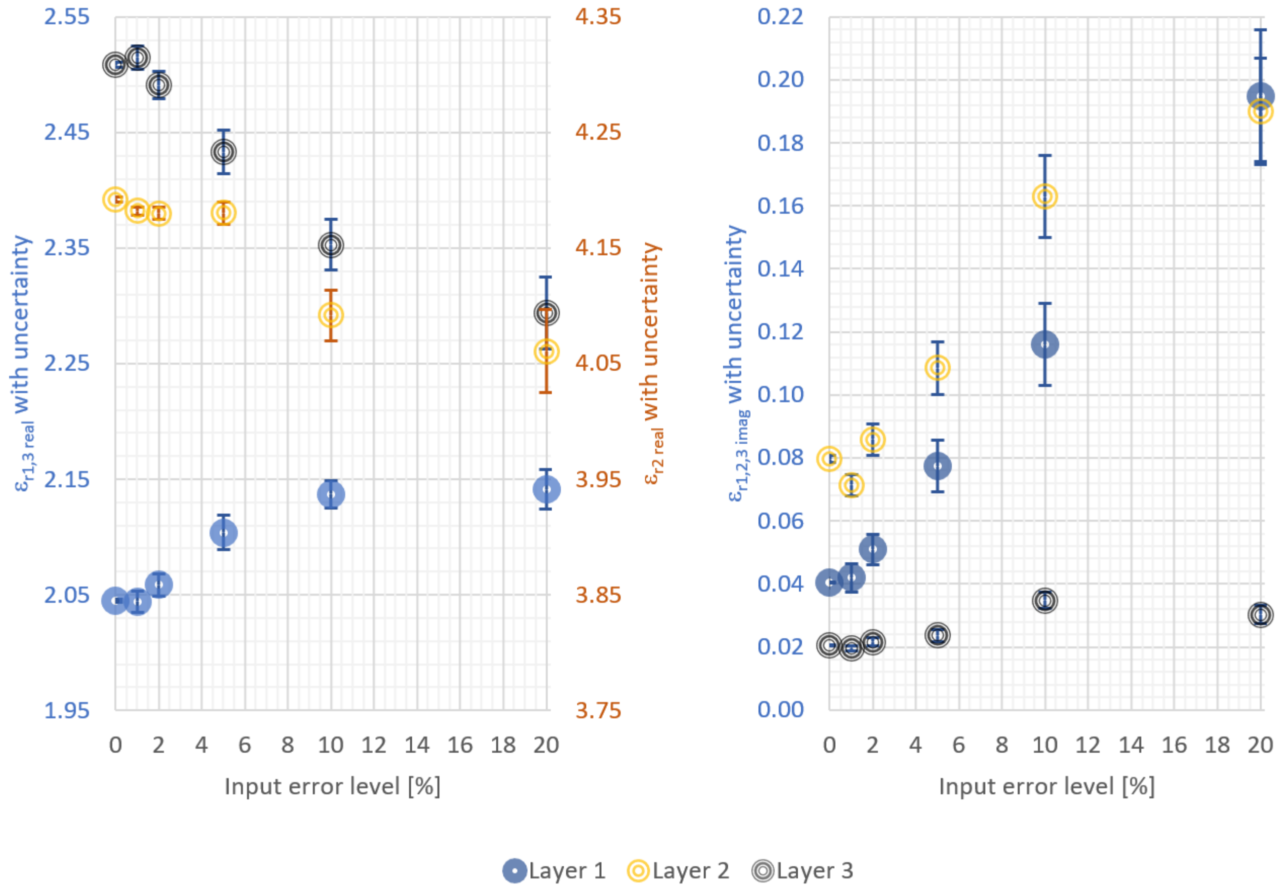

Fig. 6.1 Visualisation of the average estimated real and imaginary parts of the ϵ_r^* of a 3-layered structure with quantified uncertainties of the test case of 100 repetitions, 201 frequency points

6.3 Summary of the Uncertainty & Sensitivity Analysis

The fact that the deviations from the true (expected) value and uncertainties rise with the RSD of the input error is without a surprise. However, RSD of 20 % of the input error does not lead to similar deviation of the estimations from the expected true value. This relates to the single layer case as well as to the most complicated case represented by a structure containing 3 layers of unknown materials (6-dimensional MOP).

Considering the simplest case, a single layer with 201 input frequency points, the input error RSD of 20 % resulted in a relative deviation of 2.02 % of the final estimated mean (comparing the absolute values of the estimated mean and the true complex relative permittivity). This is a good result. However, it is even much better in the case of 402 input frequency points (as expected). The deviation is only 0.37 % in this case.

Comparing the absolute values of complex relative permittivities of the estimated mean and the true value (in the case of the input error with RSD of 20 %) the results are still acceptable. The relative deviations of the final estimations are 4.85 %, 3.22 % and 8.23 % (for the first, the second and the third layer respectively) in the case of 201 frequency points in the input. Running the software with 402 input frequency points it results in 6.49 %, 3.41 % and 7.83 %. Therefore, this is an example in which the softer granularity of the input data did not lead to results closer to the true value. However, from the pragmatical point of view, it is still surprising that the software can achieve reasonable results at all considering the high dimensionality of the problem.

7 CONTRIBUTIONS OF THE THESIS

Nowadays, the way of how to compute the transmission and reflection coefficients of a known non-magnetic homogeneous isotropic material (or several layers of known materials) at specific frequency range is already known and documented. Work presented in this statement is based on this knowledge and the inner direct model of designed system is based on it. This direct model in combination with PSO produces reasonable estimations of complex permittivity with rather low uncertainties and low sensitivity on the error of the input data. This is a non-trivial inverse task which is not presented yet in the science to date as far as the author knows. Therefore, the novel approach presented in this work may be evaluated as contributive to science also with respect to the functional and verified implementation of the designed system.

The implemented software represents one of the main contributions of this work. The software is ready to use and is capable of running in the following three modes:

1. estimation of relative permittivity/permittivities of a single or a multi-layered structure,
2. synthesis of S-parameters of a single or a multi-layered structure, and
3. estimation of relative permittivity/permittivities of a single or a multi-layered structure with addition of a noise of the normal distribution and specified standard deviation to the input S-parameters.

Another remarkable innovation in this work is the move in frequency band used for measuring and processing. This area (millimetre and sub-millimetre waves) is new also for known materials what means another breakthrough. Shift in frequencies brings also some complications. One of them is the resonance. For example the resonance of the molecules of water vapour appears near 183.310 GHz [9, 15].

It is expectable that the approaches designed in the doctoral thesis may be acknowledged primarily in the area of material physics and electrotechnics. However, it may be also applicable in the remote measurements, analysis of materials in cosmos (like measuring the thickness of specific materials, glaciers for instance) what represents a great potential of impact.

This type of research may become important in the industry in the near future for its capability to estimate properties of very new materials. This is also the area where the Department of Electronics and Measurement of Tomas Bata University in Zlín may have a chance to contribute and play an important role in terms of its laboratories' equipment and expert staff with up-to-date know-how.

8 CONCLUSIONS

The doctoral thesis briefly presented in this statement describes a specific approach aimed at estimation of complex permittivity of single or multi-layered structures of non-magnetic homogeneous isotropic materials. Its processing is based on data obtained by measuring the transmission and reflection coefficients using horn antennas in free space in the frequency range above 1 GHz. The proposed solution is presented by a working combination of a direct model computing transmission and reflection coefficients from known permittivity of layered structure under test and the Particle Swarm Optimization. This method is unusual and quite difficult to arrange due to the inverse (and thus non-deterministic) nature of this problem.

The direct mathematical model in combination with the selected evolutionary algorithm plays a significant role in the whole system and makes it possible to estimate complex permittivity of materials in multi-layered structures. Several experiments prove that this system provides reasonable estimations. Moreover, the speed of the system implemented in C++ is rather fast.

The designed system is open for further improvements as well as for changing the focus from permittivity onto another material property.

The reflection of the research objectives follows:

- A direct mathematical model computing reliable S-parameters of a known material and of a multi-layered structure of materials in free space at specific frequency ranges has been designed on the basis of the up-to-date scientific publications available at the moment.
- The direct mathematical model has been implemented into a software using C++.
- The direct mathematical model has been verified by comparing its synthetic data and data obtained by direct measurements.
- An EA (PSO) has been implemented into the software and combined with the direct mathematical model.
- Many experiments with synthetic data and real (measured) data were performed; said experiments confirm the ability of the developed system to estimate complex relative permittivity of unknown single and multi-layered structures.
- The uncertainty analysis along with the sensitivity analysis of the software has been elaborated and presented in the form of tables and figures.

In conclusion, the doctoral thesis fulfils all the required objectives.

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CPU	Central Processing Unit
EA	Evolutionary Algorithm
FR	Flame Retardant
GNU	GNU is Not Unix
GPL	General Public Licence
MOP	Multi-Objective Optimization Problem
POPOT	POPulation based Optimization Toolbox
PRNG	Pseudorandom Number Generator
PTFE	Polytetrafluoroethylene
RF	Radio Frequency, from 3 kHz to 300 GHz
RMS	Root Mean Square
RSD	Relative Standard Deviation
S-Parameters	Scattering Parameters
SI	International System of Units
VNA	Vector Network Analyser
V-Band	The electromagnetic spectrum from 40 to 75 GHz

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