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Advantages of a Multi-Frequency Experiment for Determining the Dielectric Constant of a Layer in a Rectangular Waveguide and Free Space

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Key Points:

- The well-posedness of determining the inclusion parameters by single- and multi-frequency experiments is verified
- Convergence conditions for the least squares method are established
- Estimates of the optimal experimental parameters are found

Abstract

An inverse problem of reconstructing real permittivity of a plane-parallel layer in a perfectly conducting rectangular waveguide or in free space from experimental data using an explicit expression for the scattering matrix is considered. In general, this problem is improperly posed and may be unsolvable due to inaccuracy of the experimental data, and for a perfect noiseless experiment the solution may be not unique because the scattering coefficients curve has self-intersection points. It is shown that the traditional multi-frequency method of measurements applied in vector network analyzers can be justified. The following facts are rigorously proved in the paper: nonuniqueness of the solution can be removed if the frequency resolution is sufficiently small; and an algorithm for processing measurement results using least squares provides an approximate solution to the problem that converges to the exact one when the quality of the experiment improves, the convergence rate depends on the number of frequencies used in the experiment.

1 Introduction

Knowledge of the properties of dielectrics is critical for numerous applications in material science, microwave engineering, and beyond. This is a crucial issue for developing and improving modern measurement technology and techniques implemented in advanced vector network analyzers (Rhode & Schwarz, 2012).

The known resonant and non-resonant methods for determining electrodynamic properties of materials employ mathematical models of the propagation of electromagnetic waves in the following devices: capacitors, open, volume and ring resonators (Chen et al. 2004), as well as more widely applicable devices for measuring the transmission of electromagnetic waves through a sample in free space or in a rectangular waveguide (Rothwell et al. 2016). Their use is based on an explicit formula (Nicolson and Ross, 1970) relating complex permittivity and permeability of the sample and the scattering matrix elements specifying the reflection and transmission. Due to the properties of the functions of one or several complex variables entering the reconstruction formulas, this algorithm has phase ambiguity. In (Weir, 1974) it was proposed to use a multi-frequency approach to remove the non-uniqueness using a finite-difference approximation of the solution phase derivative on the frequency mesh. However, it was not taken into account that this algorithm is unstable when inaccurate experimental data are applied.

In this paper, we attempt to overcome this drawback and develop a method employing a version of the NRW formula that couples the transmission coefficient of an electromagnetic wave with the real

dielectric constant of a lossless layer in a waveguide and in free space. We study the well-posedness condition for the inverse problem of determining the layer parameters from this formula; namely, the existence and uniqueness of solution and its continuous dependence on the input data. Unfortunately this algorithm is improperly posed. In fact, (a) the range of the function specifying the transmission coefficient is a curve on the complex plane (has the zero measure); therefore the probability that the experimental data belongs this curve is equal to zero; and (b) the parametric curve of the function on the complex plane has self-intersection points which means that the solution may not be unique.

We show that the traditional multi-frequency method of measurements realized in vector network analyzers can be modified so that ill-posedness of determining the dielectric constant of a lossless sample can be removed. In fact, for the single-frequency case, the transmission coefficient is a (scalar) function which is one-to-one if the quantity equal to the ratio of the layer width to one half of the wavelength in the layer is less than 1. In the multi-frequency case, when a vector function on a multiple frequency set is applied, a sufficient condition for the problem well-posedness is that the difference between the values of the quantity defined above at the adjacent frequencies is less than 1; for a more detailed explanation, we refer to Proposition 1 and formulas (11) and (12) below. This can be achieved by reducing the frequency resolution taking into account *a priori* estimate of the desired value of the dielectric constant. Therefore, the solution of the inverse problem is unique for a noiseless experiment that perfectly matches the mathematical model.

For an actual physical experiment, the least squares method (LSM) can be applied for the solution of the inverse problem under study. The LSM solution converges to the desired value of the layer permittivity if the quality of the experiment (determined both by noise and defects of the measurement setup and material samples) is improved. The convergence rate is enhanced if the number of frequencies used in experiment is taken large enough.

2 Problem settings

We study the problem of determining permittivity of a dielectric inclusion (a layer) in a standard rectangular waveguide (a measurement setup is displayed in Fig. 1) from the elements of the scattering matrix or the transmission coefficient of the principal waveguide mode.

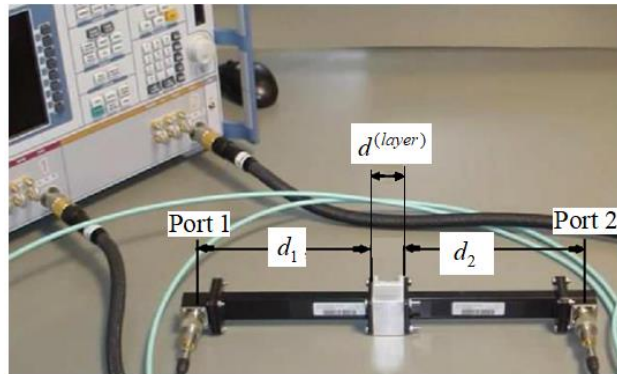


Figure 1. Rectangular waveguide with a layer (Tomasek et al., 2015).

The measurement data registered at the layer boundaries have the form (Nicolson et al., 1970)

$$S_{11}^{(layer)} = (1 - Z^2)\Gamma / (1 - \Gamma^2 Z^2), \quad (1)$$

$$S_{12}^{(layer)} = (1 - \Gamma^2)Z / (1 - \Gamma^2 Z^2), \quad (2)$$

while the values of the scattering matrix elements measured at the waveguide flanges and calculated from the complex amplitude of the harmonic Maxwell's equations solution $\mathbf{E}(\mathbf{r}, t) = \hat{\mathbf{E}}(\mathbf{r})e^{-i\omega t}$ are

$$S_{12}^{(wg,layer)} = S_{12}^{(layer)} Z_1 Z_2, \quad S_{11}^{(wg,layer)} = S_{11}^{(layer)} / (Z_1)^2,$$

where $\omega = 2\pi f$, f is the source frequency satisfying the condition of a single-mode waveguide:

$f^{(1,0)} < f < f^{(2,0)}$, $f^{(1,0)} = c/(2a)$, $f^{(2,0)} = 2f^{(1,0)}$, $f^{(1,0)}$, $f^{(2,0)}$ are the cutoff frequency for TE_{10} , TE_{20} modes, $f^{(2,0)} - f^{(1,0)} \approx 6.52 \cdot 10^9$ (GHz), and $c = (\varepsilon_0 \mu_0)^{-1/2}$ is the speed of light in vacuum.

In formulas (1) and (2)

$$\Gamma = (t_\varepsilon(f) - 1)/(t_\varepsilon(f) + 1), \quad t_\varepsilon(f) = k_\varepsilon^{(z)}(f)/k_1^{(z)}(f),$$

$$k_\varepsilon^{(z)}(f) = (k_\varepsilon^2(f) - (k^{(x)})^2)^{1/2}, \quad k_1^{(z)}(f) = (k_1^2(f) - (k^{(x)})^2)^{1/2},$$

$$k_\varepsilon(f) = \varepsilon^{1/2} k_1(f), \quad \lambda_\varepsilon(f) = 2\pi/k_\varepsilon(f), \quad k_1(f) = \omega/c, \quad k^{(x)} = \pi/a,$$

a is the waveguide width, $d^{(wg)}$, $d^{(layer)}$ are the waveguide and layer lengths, d_1 , d_2 are the distances between the ports (points of the source and field measurements) and the layer, $d^{(wg)} = d^{(layer)} + d_1 + d_2$, $\varepsilon = \varepsilon^{(layer)}$ is the layer relative dielectric constant, and ε_0 is the dielectric constant of vacuum;

$$Z_1(f) = e^{ik_1^{(z)}(f)d_1}, \quad Z_2(f) = e^{ik_1^{(z)}(f)d_2},$$

$$Z_0^{(wg)}(f) = e^{ik_1^{(z)}(f)d^{(wg)}}, \quad Z_0^{(layer)}(f) = e^{ik_1^{(z)}(f)d^{(layer)}}, \quad Z = Z^{(layer)}(f) = e^{ik_\varepsilon^{(z)}(f)d^{(layer)}}$$

are the phase shift values inside the waveguide.

Introduce the transmission coefficient of the principal mode in a single-mode perfectly conducting rectangular waveguide scattered by the dielectric layer

$$F(\varepsilon, f) = S_{12}^{(wg,layer)}(\varepsilon, f) / S_{12}^{(wg)}(f). \quad (3)$$

Here $S_{12}^{(wg,layer)}$ is the element of the scattering matrix corresponding to the transmission of the wave through the waveguide containing the dielectric layer and $S_{12}^{(wg)} = Z_0^{(wg)}$ is the corresponding element of the scattering matrix for an empty waveguide.

In the presence of a dielectric insert of arbitrary shape the measurement results change due to the occurrence of, in addition to the harmonic waves in the principal mode, a countable number of evanescent waves. These are standing waves that exponentially decay along the axis of the waveguide.

The transmission coefficient of the principal mode through a lossless dielectric layer can be found as

$$F(\varepsilon, f) = Z_0^{(layer)}(f) / g(\varepsilon, f), \quad (4)$$

where

$$g(\varepsilon, f) = c_\varepsilon(f) + iH(t_\varepsilon(f))s_\varepsilon(f), \quad (5)$$

$$s_\varepsilon(f) = \sin(k_\varepsilon^{(z)}(f)d^{(layer)}), \quad c_\varepsilon(f) = \cos(k_\varepsilon^{(z)}(f)d^{(layer)}), \quad (6)$$

and $H(x) = 0.5(x + 1/x)$, $x > 0$.

Along with the problem for the layer in a waveguide, we consider a similar problem for the layer in free space as a limiting case ($a \rightarrow \infty$) of the first setting, when

$$k^{(x)} = 0, \quad k_\varepsilon^{(z)}(f) = k_\varepsilon(f), \quad k_\varepsilon(f) = \varepsilon^{1/2} k_1(f), \quad t_\varepsilon(f) = \varepsilon^{1/2}, \quad (7)$$

105 $n=1,...,N^{(\text{exp})}$, $N^{(\text{exp})}$ is the number of frequencies used in the experiment, and (4) is the explicit formula
 106 of the transmission coefficient of the principal mode through an infinite lossless dielectric layer with

$$g(\varepsilon, f) = c_\varepsilon(f) + iH(\varepsilon^{1/2}) s_\varepsilon(f), \quad (8)$$

$$s_\varepsilon(f) = \sin(k_\varepsilon(f)d^{(\text{layer})}), c_\varepsilon(f) = \cos(k_\varepsilon(f)d^{(\text{layer})}). \quad (9)$$

107 Formula (4) together with expressions (5), (6) or (8), (9) constitute the exact solution (obtained
 108 from Maxwell's equations) for the transmission coefficient of the principal mode for both the waveguide
 109 containing a layer and an infinite layer in free space, with a distinction in determining the wavenumbers; a
 110 recurrent formula generalizing (4) to the case of a multilayer inclusion is given in (Shestopalov et al.,
 111 2015). They are equivalent to expressions (3), (2) known since 1970 (Nicolson et al., 1970), where
 112 representations (1), (2) enter the NRW formulas. According to these formulas complex parameters of a
 113 slab are determined explicitly from the scattering matrix elements $S_{11}^{(\text{layer})}$, $S_{12}^{(\text{layer})}$ using the expressions

$$\varepsilon_1 = (c_2 / c_1)^{1/2}, \quad \mu_1 = (c_1 c_2)^{1/2},$$

$$c_1 = (1 + \Gamma)^2 / (1 - \Gamma)^2, \quad c_2 = -(c \ln Z / (\omega d^{(\text{layer})}))^2,$$

$$V_1 = S_{12}^{(\text{layer})} - S_{11}^{(\text{layer})}, \quad V_2 = S_{12}^{(\text{layer})} + S_{11}^{(\text{layer})}, \quad X = (1 - V_1 V_2) / (V_1 - V_2),$$

$$\Gamma = X \pm (X^2 - 1)^{1/2}, \quad Z = (V_1 - \Gamma) / (1 - V_1 \Gamma).$$

118 Due to the properties of function $\ln z$ of a complex variable z , this algorithm has phase ambiguity.
 119 The ambiguity was removed in (Weir, 1974) using the data taken at several frequencies to find the average
 120 group delay through the sample by means of finite-difference approximation of the derivative of the phase
 121 Z with respect to f . Another difficulty of this algorithm is that it is not stable due to instability of
 122 approximate differentiation employing inaccurate data.

123 Using this example we show how the properties of a multi-frequency approach can be used to
 124 solve inverse problems, which is a goal of this study. Next, we discuss an alternative to the NRW method
 125 for determining the value of the dielectric constant of an inclusion solely from the transmission coefficient
 126 (3), (4). An advantage of the multi-frequency experiment for solving this improperly posed inverse
 127 problem using the approach developed in this work is as follows: with a sufficiently small frequency step
 128 the problem becomes properly posed for an experiment that perfectly matches the mathematical model,
 129 and the solution found by LSM approximates the desired value of the dielectric constant of the sample
 130 when the quality of a physical experiment is improved.

131 3 Algorithms of Experimental Data Processing

132 Introduce the vectors

$$\mathbf{f} = \{f_n\}_{n=1,...,N^{(\text{exp})}} \in \mathbb{R}^{N^{(\text{exp})}}, \quad \mathbf{F}^{(\text{exp})} = \{F_n^{(\text{exp})}\}_{n,...,N^{(\text{exp})}} \in \mathbb{C}^{N^{(\text{exp})}}$$

134 of the frequency and complex-valued measurement data of $N^{(\text{exp})}$ experiments. Consider the equation

$$\mathbf{g}(\varepsilon^{(\text{layer})}, \mathbf{f}) = \mathbf{g}^{(\text{exp})}, \quad (10)$$

135 for the (unknown) dielectric constant of the layer $\varepsilon^{(\text{layer})} \geq 1$, where

$$\mathbf{g}(\varepsilon, \mathbf{f}) = (g(\varepsilon, f_1), ..., g(\varepsilon, f_{N^{(\text{exp})}})) \in \mathbb{C}^{N^{(\text{exp})}}$$

136 with g defined in (5), (6), or (8), (9),

$$\mathbf{g}^{(\text{exp})} = (g_1^{(\text{exp})}, ..., g_{N^{(\text{exp})}}^{(\text{exp})}) \in \mathbb{C}^{N^{(\text{exp})}},$$

$$g_n^{(\text{exp})} = Z_0^{(\text{layer})}(f_n) / F_n^{(\text{exp})}, \quad n = 1, ..., N^{(\text{exp})}.$$

We formulate inverse problems that constitute different permittivity reconstruction scenarios of the layer in free space. To this end, let

$$\Omega^{(\varepsilon)} = \{\varepsilon : \varepsilon \geq 1\}, \quad \Omega_E^{(\varepsilon)} = \{\varepsilon : 1 \leq \varepsilon \leq E\},$$

$E > 1$, and by

$$G(\mathbf{f}, \Omega^{(\varepsilon)}) = \{ \mathbf{g}(\varepsilon, \mathbf{f}) \in \mathbb{C}^{N^{(\text{exp})}}, \varepsilon \in \Omega^{(\varepsilon)} \}$$

denote the set of values of function $\mathbf{g}(\varepsilon, \mathbf{f})$ for the selected frequency vector \mathbf{f} (it is a curve in $N^{(\text{exp})}$ -dimensional complex space).

Problem 1

Find a real $\varepsilon^{(\text{layer})} \in \Omega^{(\varepsilon)}$ satisfying relation (10) for a given complex vector $\mathbf{g}^{(\text{exp})} \in G(\mathbf{f}, \Omega^{(\varepsilon)})$ with the selected frequency vector \mathbf{f} .

Problem 2

Find a real $\varepsilon^{(\text{layer})} \in \Omega^{(\varepsilon)}$ satisfying relation (10) for a given complex vector $\mathbf{g}^{(\text{exp})} \in \mathbb{C}^{N^{(\text{exp})}}$ with the selected frequency vector \mathbf{f} .

Check the fulfillment of the well-posedness condition for these problems; namely, the existence and uniqueness of solution and its continuous dependence on the input data. Problem 1 describes a perfect experiment exactly corresponding to the mathematical model, it is solvable by the definition of the set $G(\mathbf{f}, \Omega^{(\varepsilon)})$. However, its uniqueness may be violated. In fact, if $N^{(\text{exp})} = 1$ for any chosen frequency the solution is not unique due to the existence of a countable set $\{\varepsilon_m\}_{m=1, \dots}$, satisfying the relation $\sin(k_{\varepsilon_m}(f)d^{(\text{layer})}) = 0$ that specifies self-intersections points of curve $G(f, \Omega^{(\varepsilon)})$ (see Fig. 2).

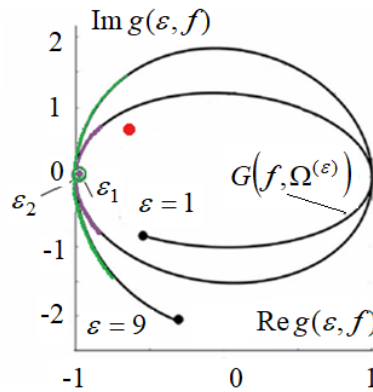


Figure 2. The branches of the curve $G(f, \Omega^{(\varepsilon)})$, $f = 9.25$ GHz, $\Omega^{(\varepsilon)} = \{\varepsilon : 1.0 \leq \varepsilon \leq 9.0\}$, corresponding to $\varepsilon \in \Omega_1^{(\varepsilon)} = (2.05, 2.13)$ (purple), $\varepsilon \in \Omega_2^{(\varepsilon)} = (3.06, 3.12)$ (green), their intersection point $g(\varepsilon_1, f) = g(\varepsilon_2, f)$, $\varepsilon_1 = 2.09 \in \Omega_1^{(\varepsilon)}$, $\varepsilon_2 = 3.12 \in \Omega_2^{(\varepsilon)}$, \bullet $g^{(\text{exp})}$.

Using *a priori* information about $\varepsilon^{(\text{layer})}$ we can achieve the uniqueness of solution by adjusting domain $\Omega_E^{(\varepsilon)}$ and a frequency range $[f_1, f_{N^{(\text{exp})}}]$. However, the formally properly posed problem may be ill-conditioned in the vicinity of the intersection points mentioned above where the parameter values are such that the quantity $\sin(k_{\varepsilon}(f)d^{(\text{layer})})$ in the denominator virtually vanishes.

Proposition 1 below demonstrates that the solution to Problem 1 is unique if the frequency resolution is sufficiently small. In fact, $\mathbf{g}(\varepsilon, \mathbf{f})$ becomes a one-to-one vector function of real variable ε for a fixed set of frequency values \mathbf{f} .

Problem 2 simulates the processing of noisy experimental data. This problem is also improperly posed since it may be unsolvable: in actual experiments, it is typical that $\mathbf{g}^{(\text{exp})} \notin G(\mathbf{f}, \Omega^{(\varepsilon)})$ because the set (a curve) has the zero measure on the complex plane. We will replace Problem 2 with an LSM problem such that its solution approximates the sought solution of perfect Problem 1 when the defects of the experimental setup and measurement error decrease.

4 One-to-One Correspondence

We consider the problem of determining the value of the dielectric constant of the lossless inclusion assuming that this quantity is real (not complex). One can show that the transition from a single-frequency experiment to a multi-frequency one improves the properties of the inverse problem providing its unique solvability. The following statement is valid both for the cases of waveguide and free space; the proof will be given for the second case to clarify major ideas of the approach.

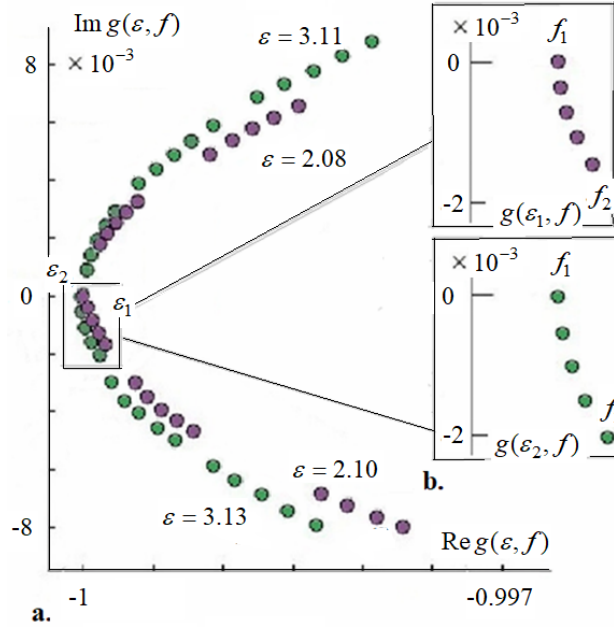


Figure 3. a. The vectors $\left(g(\varepsilon_{1,l}, f_1), \dots, g(\varepsilon_{1,l}, f_{N^{(\text{exp})}})\right), \left(g(\varepsilon_{2,l}, f_1), \dots, g(\varepsilon_{2,l}, f_{N^{(\text{exp})}})\right), N_{\text{exp}} = 5, f_1 = 9.25 \text{ GHz}, f_{N^{(\text{exp})}} = 9.2504 \text{ GHz}, \varepsilon_{1,l} \in \Omega_1^{(\varepsilon)}, \varepsilon_{2,l} \in \Omega_2^{(\varepsilon)}, l = 1, \dots, \varepsilon_{1,3} = \varepsilon_1 = 2.09, \varepsilon_{2,4} = \varepsilon_2 = 3.12$ (Figure 2), **b.** $g(\varepsilon_1, f_1) = g(\varepsilon_2, f_1), g(\varepsilon_1, f_n) \neq g(\varepsilon_2, f_n), n = 2, \dots, N^{(\text{exp})}, \rightarrow \mathbf{g}(\varepsilon_1, \mathbf{f}) \neq \mathbf{g}(\varepsilon_2, \mathbf{f})$.

Proposition 1

Set $N^{(\text{exp})} = 1$. For any $E > 1$ there is one-to-one correspondence between $\Omega_E^{(\varepsilon)}$ and $G(f, \Omega_E^{(\varepsilon)})$ for the selected frequency f if

$$\frac{d^{(\text{layer})}}{0.5\lambda_E(f)} < 1. \quad (11)$$

193 Assume that $N^{(\text{exp})} \geq 2$. For any $E > 1$ there is one-to-one correspondence between $\Omega_E^{(\varepsilon)}$ and
 194 $G(\mathbf{f}, \Omega_E^{(\varepsilon)})$ for the selected frequency vector \mathbf{f} if the following condition is satisfied in at least one of the
 195 two equivalent forms:

$$\frac{d^{(\text{layer})}}{0.5\lambda_E(f_{n+1})} - \frac{d^{(\text{layer})}}{0.5\lambda_E(f_n)} < 1, \quad (12)$$

196 $n = 1, \dots, N^{(\text{exp})} - 1$, or

$$h^{(f)} < h_E^{(f)} = \frac{c}{2d^{(\text{layer})}} \frac{1}{E^{1/2}}. \quad (13)$$

197 **Proof**

198 For $N^{(\text{exp})} = 1$ the proof is trivial. Now suppose $N^{(\text{exp})} \geq 2$. We show that if (13) holds then curve
 199 $G(\mathbf{f}, \Omega_E^{(\varepsilon)})$ has no self-intersection points (reductio ad absurdum). Let $\varepsilon_1, \varepsilon_2$ be such values of the
 200 dielectric constant of the layer that $1 \leq \varepsilon_1 < \varepsilon_2 \leq E$, $\|\mathbf{g}(\varepsilon_1, \mathbf{f}) - \mathbf{g}(\varepsilon_2, \mathbf{f})\|^{(\text{exp})} = 0$. Then the following
 201 relations

$$\begin{aligned} 202 \quad & (c_{\varepsilon_1}(f_n) - c_{\varepsilon_2}(f_n))^2 = 0, \\ 203 \quad & (H(\varepsilon_1^{1/2})s_{\varepsilon_1}(f_n) - H(\varepsilon_2^{1/2})s_{\varepsilon_2}(f_n))^2 = 0, \end{aligned}$$

204 hold for $n = 1, \dots, N^{(\text{exp})}$ due definition (4), (8), (9). Next, all the relations

$$\begin{aligned} 205 \quad & c_{\varepsilon_1}(f_n) = c_{\varepsilon_2}(f_n), \quad |s_{\varepsilon_1}(f_n)| = |s_{\varepsilon_2}(f_n)|, \quad s_{\varepsilon_1}(f_n) = \pm s_{\varepsilon_2}(f_n), \quad H(\varepsilon_1^{1/2})s_{\varepsilon_1}(f_n) = H(\varepsilon_2^{1/2})s_{\varepsilon_2}(f_n), \\ 206 \quad & \text{and therefore one of the equalities} \end{aligned}$$

$$(H(\varepsilon_2^{1/2}) - H(\varepsilon_1^{1/2}))s_{\varepsilon_1}(f_n) = 0, \quad (14)$$

207 or

$$(H(\varepsilon_2^{1/2}) + H(\varepsilon_1^{1/2}))s_{\varepsilon_1}(f_n) = 0 \quad (15)$$

208 hold for the same values n . The function $H(x) = 0.5(x + 1/x) \geq 1$ is increasing for $x \geq 1$, so the
 209 inequalities

$$210 \quad H(\varepsilon_2^{1/2}) - H(\varepsilon_1^{1/2}) > 0, \quad H(\varepsilon_2^{1/2}) + H(\varepsilon_1^{1/2}) > 0$$

211 are valid. Then $s_{\varepsilon_1}(f_n) = 0$ for $n = 1, \dots, N^{(\text{exp})}$, that is, the set of values $\{f_n\}_{n=1, \dots, N^{(\text{exp})}}$ belongs to the set of

212 zero points $\{f_m^{(0)}\}_{m=1, \dots}$ of the function $s_{\varepsilon_1}(f)$, $f_m^{(0)} = \frac{c}{2\varepsilon_1^{1/2}d^{(\text{layer})}}m$, with their number $N_0^{(f)}$ in the
 213 closed interval $[f_1, f_{N^{(\text{exp})}}]$ satisfying

$$214 \quad N_0^{(f)} \leq N_E = 2E^{1/2}d^{(f)}d^{(\text{layer})}/c + 1.$$

215 Further if (13) holds then

$$N_E < N^{(\text{exp})},$$

216 $N^{(\text{exp})} = d^{(f)}/h^{(f)} + 1$, and there are

$$N^{(\text{exp})} - N_0^{(f)} > 0 \quad (16)$$

frequency values of set $\{f_n\}_{n=1,\dots,N^{(\text{exp})}}$, such that $s_{\varepsilon_1}(f_n) \neq 0$, equality (15) is impossible, and due to (14)
 $H(\varepsilon_2^{1/2}) = H(\varepsilon_1^{1/2})$, $\varepsilon_2 = \varepsilon_1$ (a contradiction). ■

Corollary

To satisfy inequality (16) and therefore to obtain a one-to-one vector function, it is sufficient to
take $N^{(\text{exp})} = 2$, $f_{N^{(\text{exp})}} = f_1 + h^{(f)}$ for any f_1 with $h^{(f)}$ satisfying inequality (13), $d^{(f)} = h^{(f)}$; if interval
 $d^{(f)}$ is given then the smallness of the frequency step $h^{(f)}$ is provided by the choice of a sufficiently large
number of frequencies $N^{(\text{exp})}$.

If an *a priori* estimate for the range of values of the sample permittivity is known then the
following conclusions are valid: (i) condition (11) shows that for the single-frequency case, the solution to
Problem 1 is unique for a sufficiently narrow layer whose width is less than one half of the wavelength in
the layer; (ii) in the multi-frequency case, the well-posedness condition (12) or (13) can be fulfilled for a
layer of any width by reducing the frequency step (Figure 3).

Example

If the conditions of Proposition 1 are violated, we give two examples of self-intersection of
parametric curves $G(f, \Omega^{(\varepsilon)})$ and $G(\mathbf{f}, \Omega^{(\varepsilon)})$. Let $\varepsilon_m^{1/2} = E^{1/2} m/2 \leq E^{1/2}$, $m = 1, 2$. Then

$$k_{\varepsilon_m}(f) d^{(\text{layer})} = \pi n \text{ and } g(\varepsilon_m, f) = (-1)^m \text{ if } N^{(\text{exp})} = 1 \text{ and } \frac{d^{(\text{layer})}}{0.5\lambda_E(f)} = 2 \text{ contrary to (11);}$$

$$k_{\varepsilon_m}(f_n) d^{(\text{layer})} = \pi m \text{ and } g(\varepsilon_m, f_n) = (-1)^{mn}, \text{ if } N^{(\text{exp})} \geq 2 \text{ and } f_n = nh^{(f)}, n = 1, \dots, N^{(\text{exp})},$$

$$h^{(f)} = 2h_E^{(f)} \text{ contrary to (13).}$$

Consider the function

$$S(\varepsilon, N^{(\text{exp})}, \mathbf{f}, d^{(\text{layer})}) = \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} s_{\varepsilon}^2(f_n),$$

where $f_n = f_1 + (n-1)h^{(f)}$, $n = 1, \dots, N^{(\text{exp})}$, s_{ε} , $k_{\varepsilon}^{(z)}$ are defined by (6), (7) for the case of a slab in free
space. We now prove an important auxiliary statement.

Proposition 2

For $\varepsilon \in \Omega_E^{(\varepsilon)}$, $E \geq 1$, and $h^{(f)}$ satisfying condition (13) the following inequalities hold:

a.

$$S(\varepsilon, N^{(\text{exp})}, \mathbf{f}, d^{(\text{layer})}) \geq \underline{S}(d^{(\text{layer})} h^{(f)}) > 0, \quad (17)$$

$$\text{where } \underline{S}(x) = 2x^2 / c^2;$$

b.

$$S(\varepsilon, N^{(\text{exp})}, \mathbf{f}, d^{(\text{layer})}) \geq 0.5(1 - \alpha) > 0 \quad (18)$$

for any $0 < \alpha < 1$ if

$$N^{(\text{exp})} \geq \underline{N}(d^{(\text{layer})} h^{(f)}) / \alpha \geq 0.5E^{1/2} / \alpha, \quad (19)$$

$$\text{where } \underline{N}(x) = 0.25c / x.$$

Proof

a. It is easy to verify that for any $N = 2, \dots$, $0 < h < \pi$, $x_n = x_1 + (n-1)h$, $n = 1, \dots, N$, the inequality

$$\frac{1}{N} \sum_{n=1}^N \sin^2(x_n) \geq \frac{h^2}{2\pi^2} \quad (20)$$

is true. This follows from the relation

$$\begin{aligned} \frac{1}{N} \sum_{n=1}^N \sin^2(x_n) &= 0.5 \left(1 - \frac{1}{N} \sum_{n=1}^N \cos(2x_n) \right) = \\ &= 0.5 \left(1 - \frac{1}{N} \frac{1}{\sin h} \sin(Nh) \cos(x_N + x_1) \right) \geq 0.5 \left(1 - \frac{|\sin(Nh)|}{N |\sin h|} \right), \end{aligned}$$

because

$$|\sin(nh)| \leq |\sin((n-1)h)| + |\sin h| \leq n |\sin h|,$$

$$(N-1)/N \geq 0.5,$$

$$\begin{aligned} 1 - \frac{|\sin(Nh)|}{N |\sin h|} &= \left| 1 - \left(\frac{\sin((N-1)h)}{N \sin h} \cos h + \frac{\cos((N-1)h)}{N \sin h} \sin h \right) \right| \geq \\ &\geq 1 - (|\cos h|(N-1)/N + 1/N) = (1 - |\cos h|)(N-1)/N \geq \sin^2(0.5h), \end{aligned}$$

and $\sin x \geq \frac{2}{\pi} x$ for $0 < x < \frac{\pi}{2}$.

Thus if inequality (13) holds, then

$$0.5k_\varepsilon(h^{(f)})d^{(layer)} \leq \pi/2, \quad \sin^2(0.5k_\varepsilon(h^{(f)})d^{(layer)}) \geq \sin^2(0.5k_1(h^{(f)})d^{(layer)}),$$

$k_\varepsilon(h^{(f)}) = 2\pi h^{(f)} \varepsilon^{1/2} / c$, since function $\sin x$ is monotonic at $0 < x < \pi/2$. As a result, we obtain estimate (17) for $\varepsilon \in \Omega_E^{(\varepsilon)}$ using (20) for $x_n = k_\varepsilon(f_n)d^{(layer)}$, $n = 1, \dots, N^{(\exp)}$.

b. Estimate (18) follows from the inequality $\frac{|\sin(Nh)|}{N |\sin h|} \leq \frac{\pi}{2Nh}$ which holds for $0 < h < \frac{\pi}{2}$, the

right-hand side of (19) follows from condition (13). ■

The following statement together with Proposition 1 shows that for a sufficiently small frequency resolution Problem 1 is properly posed; that is, its solution is unique and continuously depends on the input data entering the right-hand side of the equation.

Define the condition number as

$$\kappa = \sup \left(\frac{|\varepsilon_1 - \varepsilon_2|}{\|\mathbf{g}(\varepsilon_1, \mathbf{f}) - \mathbf{g}(\varepsilon_2, \mathbf{f})\|^{(\exp)}}, \{\varepsilon_1, \varepsilon_2\} \subset \Omega^{(\varepsilon)} \right), \quad (21)$$

with a norm $\|\cdot\|^{(\exp)}$ defined by $\|\mathbf{g}\|^{(\exp)} = \left(\frac{1}{N^{(\exp)}} \sum_{n=1}^{N^{(\exp)}} |g_n|^2 \right)^{1/2}$ for $\mathbf{g} = (g_1, \dots, g_{N^{(\exp)}}) \in \mathbb{C}^{N^{(\exp)}}$.

Proposition 3

If the conditions of Proposition 2 are satisfied, then the solution to Problem 1 depends continuously on the experimental data; i.e., if

$$\|\mathbf{g}(\varepsilon_1, \mathbf{f}) - \mathbf{g}(\varepsilon_2, \mathbf{f})\|^{(\text{exp})} \rightarrow 0, \quad (22)$$

for $\{\varepsilon_1, \varepsilon_2\} \subset \Omega_E^{(\varepsilon)}$, then

$$|\varepsilon_1 - \varepsilon_2| \rightarrow 0. \quad (23)$$

Proof

For the case of a slab in free space we introduce the vectors

$$\mathbf{c}_m = (c_{m,1}, \dots, c_{m,N^{(\text{exp})}}), \quad \mathbf{s}_m = (s_{m,1}, \dots, s_{m,N^{(\text{exp})}}), \quad \mathbf{d}_m = (d_{m,1}, \dots, d_{m,N^{(\text{exp})}}),$$

$$c_{m,n} = \cos(k_{\varepsilon_m}(f_n)d^{(\text{layer})}), \quad s_{m,n} = \sin(k_{\varepsilon_m}(f_n)d^{(\text{layer})}), \quad d_{m,n} = H(\varepsilon_m^{1/2})s_{m,n}, \quad m=1,2, \quad n=1, \dots, N^{(\text{exp})}.$$

Assume that

$$\|\mathbf{g}(\varepsilon_1, \mathbf{f}) - \mathbf{g}(\varepsilon_2, \mathbf{f})\|^{(\text{exp})} = \delta, \quad (24)$$

δ is small enough by assumption (22), and $1 \leq \varepsilon_m < \infty$, $m=1,2$. Due (24) the following inequalities hold:

$$\|\mathbf{c}_1 - \mathbf{c}_2\|^{(\text{exp})} \leq \delta, \quad (25)$$

$$\|\mathbf{d}_1 - \mathbf{d}_2\|^{(\text{exp})} \leq \delta. \quad (26)$$

It follows from (25) that for $m=1,2$ the norms $\|\mathbf{c}_m\|^{(\text{exp})}$, $\|\mathbf{s}_m\|^{(\text{exp})}$, $\|\mathbf{d}_m\|^{(\text{exp})}$ are pairwise close:

$$\left| \left(\|\mathbf{s}_1\|^{(\text{exp})} \right)^2 - \left(\|\mathbf{s}_2\|^{(\text{exp})} \right)^2 \right| \leq 2\delta. \quad (27)$$

In fact, using the triangle inequality we obtain the following estimates:

$$\left| \left(\|\mathbf{s}_1\|^{(\text{exp})} \right)^2 - \left(\|\mathbf{s}_2\|^{(\text{exp})} \right)^2 \right| = \left| \left(\|\mathbf{c}_1\|^{(\text{exp})} \right)^2 - \left(\|\mathbf{c}_2\|^{(\text{exp})} \right)^2 \right| = \left| \left(\|\mathbf{c}_1\|^{(\text{exp})} + \|\mathbf{c}_2\|^{(\text{exp})} \right) \left(\|\mathbf{c}_1\|^{(\text{exp})} - \|\mathbf{c}_2\|^{(\text{exp})} \right) \right| \leq$$

$$\leq 2 \left| \left(\|\mathbf{c}_1\|^{(\text{exp})} - \|\mathbf{c}_2\|^{(\text{exp})} \right) \right| \leq 2 \|\mathbf{c}_1 - \mathbf{c}_2\|^{(\text{exp})}.$$

Similarly, due to (26),

$$\left| \left(\|\mathbf{d}_1\|^{(\text{exp})} \right)^2 - \left(\|\mathbf{d}_2\|^{(\text{exp})} \right)^2 \right| \leq 2\delta. \quad (28)$$

Using the representation

$$\left| \left(\|\mathbf{d}_1\|^{(\text{exp})} \right)^2 - \left(\|\mathbf{d}_2\|^{(\text{exp})} \right)^2 \right| = \left| H^2(\varepsilon_2^{1/2}) \left(\frac{H^2(\varepsilon_1^{1/2}) - H^2(\varepsilon_2^{1/2})}{H^2(\varepsilon_2^{1/2})} \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} s_{1,n}^2 + \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} (s_{1,n}^2 - s_{2,n}^2) \right) \right|$$

and the inequalities $H^2(\varepsilon^{1/2}) \geq 1$, $\varepsilon \geq 1$, (27), (28) we have

$$\left| \frac{H^2(\varepsilon_1^{1/2}) - H^2(\varepsilon_2^{1/2})}{H^2(\varepsilon_2^{1/2})} \right| \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} s_{1,n}^2 - \left| \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} (s_{1,n}^2 - s_{2,n}^2) \right| \leq 2\delta,$$

$$\left| \frac{H^2(\varepsilon_1^{1/2}) - H^2(\varepsilon_2^{1/2})}{H^2(\varepsilon_2^{1/2})} \right| \frac{1}{N^{(\text{exp})}} \sum_{n=1}^{N^{(\text{exp})}} s_{1,n}^2 \leq 4\delta. \quad (29)$$

Further,

$$\left| \frac{H^2(\varepsilon_1^{1/2}) - H^2(\varepsilon_2^{1/2})}{H^2(\varepsilon_2^{1/2})} \right| = \frac{(\varepsilon_2 - 1/\varepsilon_1)}{(\varepsilon_2 + 1)^2} |\varepsilon_1 - \varepsilon_2| \geq \frac{(\varepsilon_2 - 1)}{(\varepsilon_2 + 1)^2} |\varepsilon_1 - \varepsilon_2|,$$

if $\varepsilon_1 \geq 1$, so that we obtain

$$|\varepsilon_1 - \varepsilon_2| \leq K_1(\varepsilon_2) \left| \frac{H^2(\varepsilon_1^{1/2}) - H^2(\varepsilon_2^{1/2})}{H^2(\varepsilon_2^{1/2})} \right|, \quad (30)$$

where $K_1(x) = \frac{(x+1)^2}{x-1}$.

From inequalities (29), (30) it follows that under the conditions of Proposition 2 the following estimates are valid:

$$|\varepsilon_1 - \varepsilon_2| \leq \kappa_1 \delta \quad (31)$$

due to (17) with $h^{(f)}$ satisfying condition (13),

$$\kappa_1 = 4K_1(\varepsilon_2)K_2(d^{(layer)}h^{(f)}), \quad (32)$$

$K_2(x) = \frac{c^2}{2x^2}$, and

$$|\varepsilon_1 - \varepsilon_2| \leq \kappa_2 \delta \quad (33)$$

due to (18) with

$$\kappa_2 = 8K_1(\varepsilon_2)/(1-\alpha), \quad (34)$$

$0 < \alpha < 1$, estimate (33) holds if to choose a sufficiently large $N^{(exp)}$ according to (19).

A consequence of (31), (33) is the estimate

$$|\varepsilon_1 - \varepsilon_2| \leq \kappa \delta, \quad (35)$$

with

$$\kappa \leq \kappa_1, \quad \kappa \leq \kappa_2.$$

Finally, inequality (35) proves the sought limiting relation (23). ■

Quantities κ_1 and κ_2 given by (32) and (34) are upper bounds for the condition number κ defined in (21). The estimate κ_1 is not the best because a small frequency step enters the denominator. The estimate κ_2 can be improved by increasing $N^{(exp)}$. Note that both estimates are no longer bounded if *a priori* values of the sought layer relative permittivity are close to 1 (vacuum) or become too large.

Thus, at any frequency f , the parametric curve representing the set of the values of function $g(\varepsilon, f)$ has a countable number of the touch points of loops in the complex plane. On the other side, the curve corresponding to the vector function $\mathbf{g}(\varepsilon, \mathbf{f}) = (g(\varepsilon, f_1), \dots, g(\varepsilon, f_{N^{(exp)}}))$ for a selected set of frequencies $\mathbf{f} = (f_1, \dots, f_{N^{(exp)}})$ in a multidimensional complex space is not self-intersecting if the measurement frequency step belongs to the admissible range which can be determined for the given parameters of the problem. Moreover, the function inverse to $\mathbf{g}(\varepsilon, \mathbf{f})$ is continuous for a fixed \mathbf{f} . For that reason Problem 1 of reconstructing the layer real permittivity from the perfect noiseless data becomes properly posed.

In the next section, we consider the LSM problem which replaces improperly posed Problem 2

313 simulating a physical experiment to search the dielectric constant of the layer in free space. A more
 314 complicated case of a layer in a waveguide was discussed in (Sheina et al., 2019).

315 **5 Multi-frequency least squares method**

316 **Problem 3 (least squares method, LSM)**

317 Find a real value $\varepsilon^{(LS)}$ satisfying the condition

$$318 \quad \left\| \mathbf{g}(\varepsilon^{(LS)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} = \min \left(\left\| \mathbf{g}(\varepsilon, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})}, \varepsilon \in \Omega_E^{(\varepsilon)} \right)$$

319 for a given complex vector $\mathbf{g}^{(\text{exp})} \in \mathbb{C}^{N^{(\text{exp})}}$ with the selected frequency vector \mathbf{f} .

320 **Proposition 4**

321 The Problems 3 is solvable.

322 **Proof**

323 This follows from Weierstrass theorem on the minimum of a continuous function on a compact
 324 set. ■

325 **Note**

326 The solution to Problem 3 may not be unique, since the parametric curve $G(\mathbf{f}, \Omega^{(\varepsilon)})$ is not convex
 327 set.

328 **Proposition 5**

329 If the conditions of Proposition 2 are satisfied and

$$\left\| \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \rightarrow 0, \quad (36)$$

330 then

$$\varepsilon^{(LS)} \rightarrow \varepsilon^{(layer)}. \quad (37)$$

331 **Proof**

332 Assume that

$$\left\| \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} = \delta,$$

333 and δ is small enough due to (36). By definition of solution to Problem 3 we have

$$\left\| \mathbf{g}(\varepsilon^{(LS)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \leq \left\| \mathbf{g}(\varepsilon, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \quad (38)$$

334 for all $\varepsilon \in \Omega_E^{(\varepsilon)}$. In particular, we can choose $\varepsilon = \varepsilon^{(layer)}$ and obtain an inequality

$$335 \quad \left\| \mathbf{g}(\varepsilon^{(LS)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \leq \left\| \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})}$$

336 that follows from (38). So

$$337 \quad \left\| \mathbf{g}(\varepsilon^{(LS)}, \mathbf{f}) - \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) \right\|^{(\text{exp})} \leq \left\| \mathbf{g}(\varepsilon^{(LS)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} + \left\| \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \leq$$

$$338 \quad \leq 2 \left\| \mathbf{g}(\varepsilon^{(layer)}, \mathbf{f}) - \mathbf{g}^{(\text{exp})} \right\|^{(\text{exp})} \leq 2\delta.$$

339 Thus (37) holds due to estimate

$$|\varepsilon^{(LS)} - \varepsilon^{(layer)}| \leq 2\kappa_2\delta \quad (39)$$

with

$$\kappa_2(\alpha) = 8 \frac{(\varepsilon^{(layer)} + 1)^2}{\varepsilon^{(layer)} - 1} \frac{1}{1 - \alpha}$$

defined in Proposition 2 by (34) for any $0 < \alpha < 1$, if

$$N^{(exp)} \geq \frac{c}{4d^{(layer)}h^{(f)}} \frac{1}{\alpha} \geq \frac{E^{1/2}}{2\alpha}$$

according to (19) and the frequency step does not exceed the admissible upper bound defined by condition (13) based on *a priori* estimate of the dielectric constant of the sample. ■

Estimate (39) shows how a small error in the measurement data affects the accuracy of the approximation of the exact value of the dielectric constant by the value determined using LSM. The estimate takes into account the effect of the size of the layer, the resolution of the frequency and the number of frequencies used in experiment.

Applying these results one can get the best possible rate of convergence of the approximate solution to the sought value by improving the quality of experimental data, as shown in Figure 4 for an actual experiment (Ivanchenko et al., 2016).

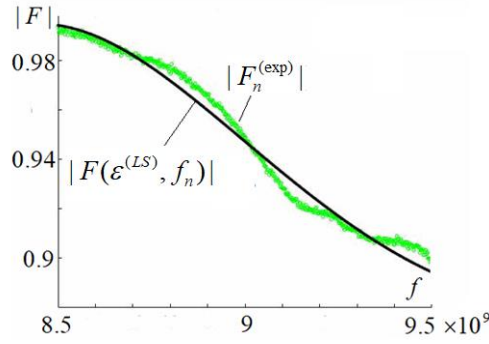


Figure 4. Data $\{|F_n^{(exp)}|\}_{n=1, \dots, N^{(exp)}}$ of an experiment with a Teflon layer (a dielectric permittivity $\varepsilon \approx 2.01-2.1$), the frequency range 8.5–9.5 (GHz) with no self-intersection points of the curve $G(f, \Omega^{(\varepsilon)})$, \searrow is $\{|F(\varepsilon^{(LS)}, f_n)|\}_{n=1, \dots, N^{(exp)}}$ calculated by LSM.

Example

The upper bounds of the admissible frequency resolution defined by (13) are $h_E^{(f)} \approx 5, 3.5, 1.6, 0.5$ (GHz) for *a priori* estimates of the dielectric constant of the inclusion $E \approx 1, 2, 10, 100$ for vacuum, Teflon, quartz, and water, respectively; $d^{(layer)} = 0.03$ (m). For quartz $E \approx 10$, $h_E^{(f)} \approx 1.6$ (GHz), and for $\alpha = 0.1$, $N^{(exp)} = E^{1/2} / 2\alpha \approx 16$, so that $K_1(E) \approx 13.4$, and $\kappa_2 \approx 30$.

6 Conclusions

We have shown how to modify the traditional multi-frequency measurement technique in order to overcome ill-posedness of reconstructing the layer permittivity in a rectangular waveguide and free space. The well-posedness can be achieved by reducing the frequency resolution taking into account an *a priori* given range of values of the dielectric constant.

The uniqueness of the resulting solution and well-posedness of the corresponding inverse problems are rigorously proved in a series of mathematical statements.

370 The developed approach leads to a practical algorithm of calculating the permittivity employing
371 LSM. The solution obtained using this algorithm converges to the sought layer permittivity with the
372 controlled rate under the condition that the quality of the experiment is improved.

373 **Acknowledgment**

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375 The data availability statement: data were not used, nor created for this research.

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Figure 1.

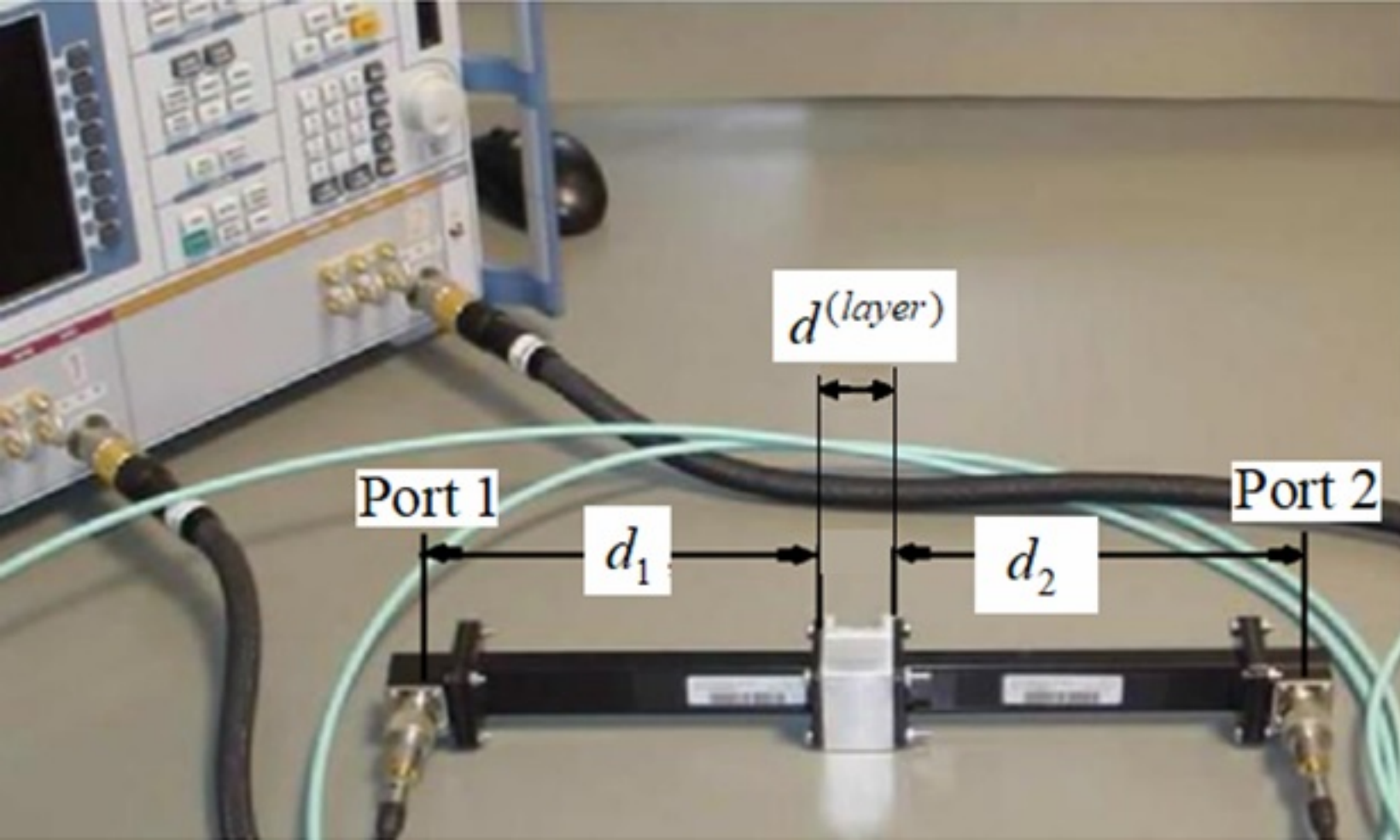


Figure 2.

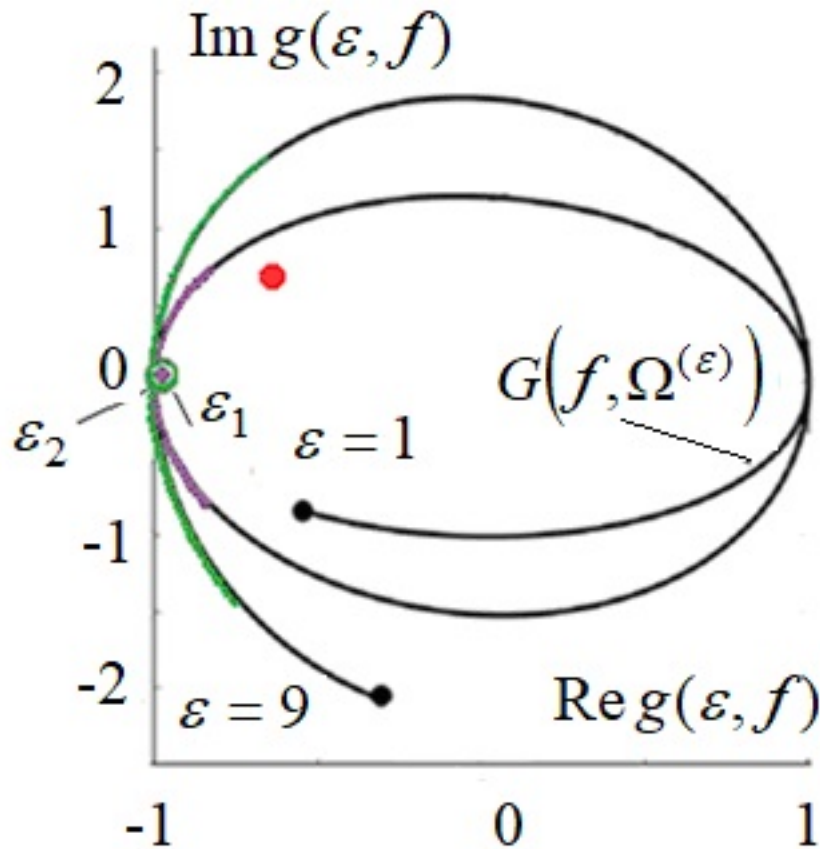


Figure 3.

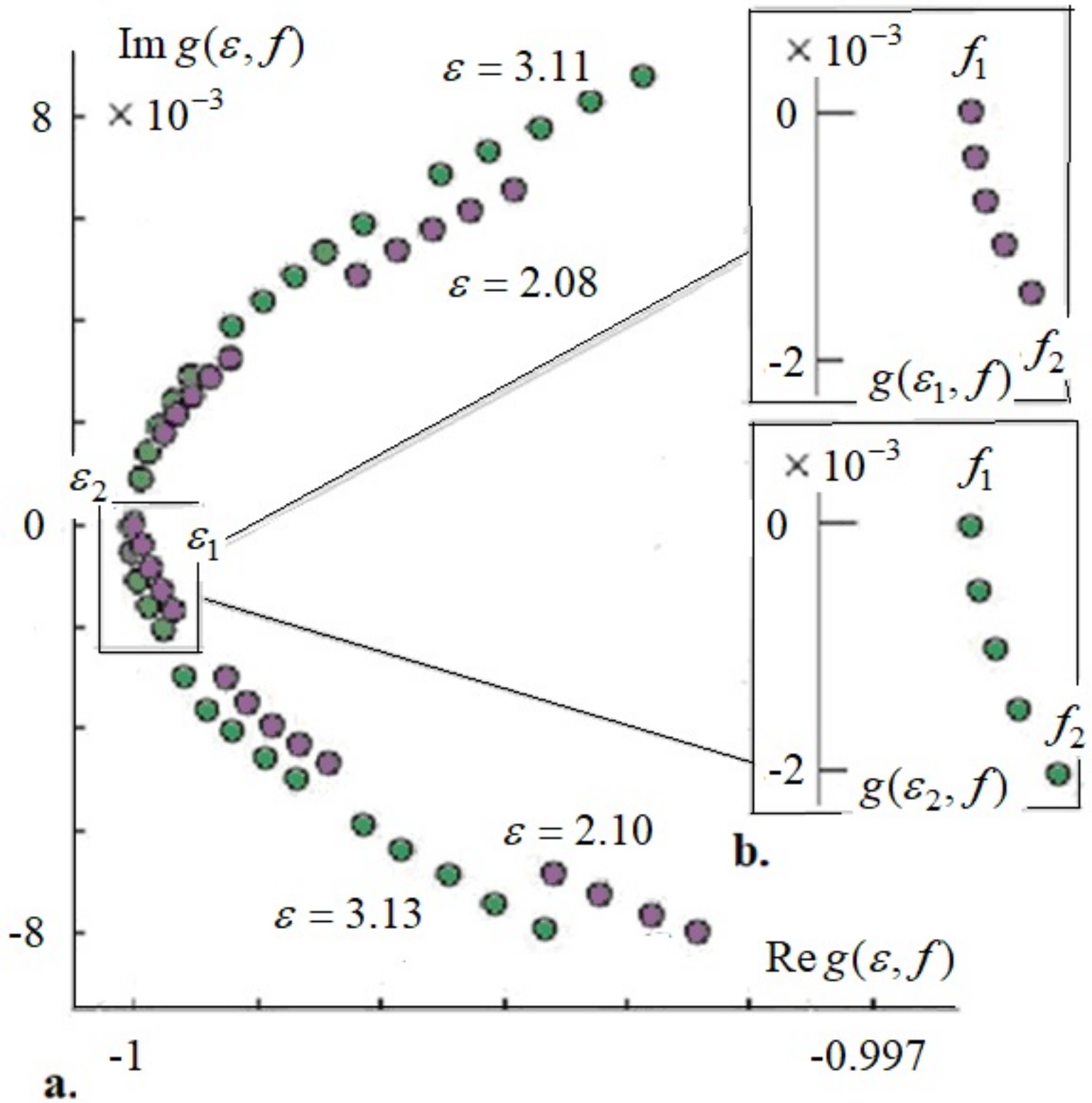


Figure 4.

