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# INVERSE SCATTERING PROBLEM IN DIAGNOSTICS OF MULTILAYER PERIODIC STRUCTURES

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## Abstract

The dual regularization method is applied in the inverse problem of electromagnetic scattering to retrieve permittivity inhomogeneities in multilayer periodic dielectric structures. Based on the developed theory, the solution algorithm has been worked out and applied in the numerical simulation of the multifrequency reflectometry diagnostics of inhomogeneities in multilayer structures of X-ray optics.

***Keywords:*** Dual regularization, inverse scattering problem, electromagnetic sounding, permittivity profile, multilayered periodic structures.

## 1. INTRODUCTION

Inverse problems of scattering are widely used in various methods of sounding and tomography of media parameters in electromagnetism, acoustics and quantum mechanics. For one-dimensional (1D) distributions of media parameters, they can be reduced to the known Gelfand-Levitan-Marchenko equation. However, this theory is inapplicable to layered or absorbing media.

In frameworks of electromagnetic perturbation theory, the inverse scattering problem in various statements can been reduced to the non-linear integral equation of the 1$^{st}$ kind that should been solved iteratively, beginning with the Born approximation [1]. Based on this equation, the one-dimensional problem has been solved with the use of Tikhonov's method of generalized discrepancy [2]. Results of the numerical study in the problem of low-frequency sounding of the Earth crust [3] have demonstrated serious limitations of such approach for large perturbations, when the Born approximation (first guess of iterative method) is inapplicable. To overcome these restrictions of perturbation theory, the new method of dual regularization based on the Lagrange approach in the optimization theory [4] has been applied [5] in this problem. Results show its ability to retrieve very strong variations of conductivity profiles.

The approach, based on the solution of the non-linear integral equation and the theory of multilayer scattering [6] has been also applied to diagnostics of permittivity inhomogeneities in multilayer periodical structures that are basic elements of the modern X-ray optics [7]. Some deviations from a desired perfect meander structure appear as a result of the material diffusivity related to the epitaxial technique used in the structures production. For diagnostics of these structures, reflectometry measurements of X-ray scattering are in use. This method has obvious advantages: it is noncontact, non-destructive and fast in comparison with the electron microscopy or SIMS (secondary ion mass-spectrometry). One-dimensional structure defects can be described in the terms of the periodic permittivity profile.

But, as it was shown in [8,9], the solution of this problem based on non-linear integral equation also has serious restrictions related to the Born approximation and linearization. Here we propose a new method of this problem solution based on the dual-regularization approach and present results of numerical simulation of the corresponding inverse scattering problem.

## 2. THEORY

### 2.1. ONE-DIMENSIONAL INVERSE PROBLEM OF SCATTERING

Following [7], consider a periodic multilayer (in $z$-direction) medium with the period $d = d_1 + d_2$ with a complex permittivity profile $\varepsilon(z) = \varepsilon'(z) + i\varepsilon''(z)$. Assuming that this profile of inhomogeneities $\varepsilon_1(z) = \varepsilon_1(z + d)$ is also periodic, it can be expressed as

$$\varepsilon(z) = \begin{cases} \varepsilon_{01},\ z < 0 \\ \varepsilon_{02} + \varepsilon_1(z),\ 2id \le z < 2id + d_1 \\ \varepsilon_{03} + \varepsilon_1(z),\ (2i+1)d \le z \le (2i+1)d + d_2 \\ \varepsilon_{04},\ z > Nd \end{cases}, \quad (1)$$

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$i = 0, 2..., N/2$. Dielectric parameters of layers are, in general, absorbing and frequency-dependent. Because $\varepsilon_1(z)$ is formed due by the mutual penetration of two components of the meander structure, it is reasonable to represent it as $\varepsilon_1(z) = f(z)(\varepsilon_{03} - \varepsilon_{02})$, where complex-valued permittivity perturbations of this mixture are determined by the real-valued profile $f(z)$.

### 2.2. Method of Dual Regularization

In the proposed reflectometry diagnostics the difference

$$\Delta r_0(\omega) = \left|R_m\right|^2 - \left|R_0\right|^2 \tag{2}$$

between the measured reflection coefficient and that, calculated by known parameters of the meander structure $d_1, d_2, N$ in dependence on frequency is in use. Then, the statement of the inverse scattering problem is formulated like this: to find such a profile $f(z)$ that the condition

$$\Delta r[f](\omega) = \left|R\right|^2[f] - \left|R_0\right|^2 = \Delta r_0(\omega)\,. \tag{3}$$

is satisfied at any frequency $\omega \in [\omega_1, \omega_2]$, where $\left|R\right|^2[f]$ is the reflection coefficients calculated for a profile *f*(*z*). This problem can be expressed as an equivalent problem of conditional minimization of the functional

$$\begin{gathered} I_0(f) \equiv \left\|f\right\|^2 \to \min, \quad \Delta r[f](\omega) = \Delta r_0(\omega), \\ f \in \mathrm{L}_2(0,d) \equiv \mathrm{D}, \quad \omega \in [\omega_1, \omega_2] \end{gathered} \tag{4}$$

The modified Lagrange functional of this problem is:

$$\begin{aligned} L_\mu(f, x_0, \lambda) &\equiv \| f \|^2 \\ &+ \int_{\omega_1}^{\omega_2} \lambda(\omega)\left(\Delta r[f](\omega) - \Delta r_0(\omega)\right)d\omega \\ &+ \mu\Big(\sqrt{\int_{\omega_1}^{\omega_2} \left(\Delta r[f](\omega) - \Delta r_0(\omega)\right)^2 d\omega} \\ &\quad + \int_{\omega_1}^{\omega_2} \left(\Delta r[f](\omega) - \Delta r_0(\omega)\right)^2 d\omega\Big), \end{aligned} \tag{5}$$

and the corresponding regularized modified dual problem:

$$\begin{gathered} V_\mu^\alpha = V_\mu(\lambda) - \alpha \| \lambda \|^2 \equiv \\ \min_{(f, x_0) \in \mathrm{R}^4 \times \mathrm{L}_2(0, z_n)} L_\mu(f, \lambda) - \alpha \| \lambda \|^2 \to \max, \\ \lambda \in \Lambda_\mu \equiv \{\lambda \in \mathrm{L}_2(\omega_1, \omega_2) : \| \lambda \| \le \mu\}. \end{gathered} \tag{6}$$

where $\alpha$ is the regularization parameter, on the Hilbert space $L_2(\omega_1, \omega_2)$. The supergradient of this functional is expressed explicitly. The following scheme of the solution consists of the gradient minimization of (5) at the simultaneous maximization of (6). The function $f(z)$ in the saddle point gives us the desired regularized solution.

When the angular dependence is in use in analysis, it is enough to make obvious changes of arguments and integration variables.

## 3. Numerical Simulation

A numerical algorithm of the dual regularization method has been worked out and applied in the simulation of the proposed diagnostics of inhomogeneity profile of permittivity in multilayer structures. The numerical simulation has been carried out for inhomogeneities in the periodic Mo-Si 50-layer structure (the same as in [7]), which has been retrieved by multifrequency reflectometry data in the wavelength range $\lambda = 12.5 \div 14.5$ nm at the elevation angle $\theta = 85^0$, where TE-component dominates in scattering. As it has been shown in [7], in this spectral range the reflection coefficient has a considerable sensitivity to profile variations.

In Fig. 1, results of the numerical simulation are shown. The retrieval has been carried out using "measurement data" with errors, which have been simulated by gauss-distributed random values with *rms* $\delta r = 0{,}012$. The saddle point has been achieved at the discrepancy level 0.0118 that is very close to the level of simulated errors. At the gradient minimization of the functional (5), the natural *a priory* constraint $0 \le f \le 1$ has been in use. Permittivity is given for $\lambda = 13.3$ nm.

Retrieval results demonstrate a good agreement with parameters of initial profile with sharp gradients of permittivity at layers' interfaces.

The simulation study meets with serious difficulties related to the absence of the phase information in the reflected signal. Sometimes, the gradient minimization of (5) up to the level of simulated errors leads to a profile that is much different from the simulated one, i.e., to the false solution of the nonlinear problem that corresponds to a local minimum. But, at the following step of maximization of the dual problem functional (6), the solution can be shifted from such local minima.

To realize this advantage of the dual regularization, it is necessary to fit parameters of the iteration scheme using the available freedom of their choice, or find the solution as the deviation of a reasonably chosen first guess.

The numerical simulation shows that the algorithm convergence is much better, if such a first guess (as, for example, the solution of the corresponding linearized problem [7]) is used. This way to involve the additional *a priori* information usually leads to a much better quality of the solution in ill-posed problems.

The considered problem is so difficult that it is hardly possible to realize a universal algorithm for an arbitrary profile of inhomogeneity. In any case the reliability of the obtained solution should be studied especially in the numerical simulation.

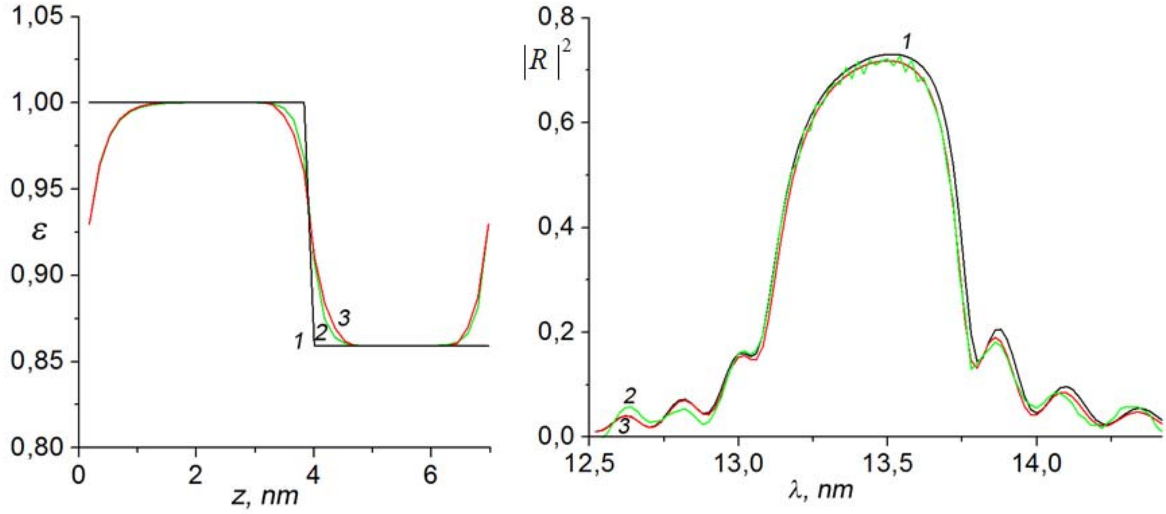


**Fig. 1.** Left: (1) meander structure, (2) initial profile of $\mathrm{Re}\,\varepsilon(z)$ ,(3) retrieved profile; Right: (1) $|R_0(\lambda)|^2$, (2) $|R_m(\lambda)|^2$, (3) $|R(\lambda)|^2$ for retrieved profile.

But, nevertheless, in the considered case of diffusive inhomogeneities, when profiles are monotone decreasing from layers' interfaces, the developed algorithm, based on the dual regularization method, gives good results in the wide enough range of possible parameters of inhomogeneities.

## 4. Permission to Publish

The authors are responsible for all material contained in the manuscript they submit. Co-authors agree to the submission of the paper.


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