INVERSE SCATTERING PROBLEM IN PSEUDOPULSE DIAGNOSTICS OF 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 by the pseudopulse synthesized from multifrequency reflectometry measurements. Based on the developed theory, the solution algorithm has been worked out and applied in the numerical simulation of this reflectometry diagnostics of inhomogeneities in multilayer structures of X-ray optics.**

I. 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 1st 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. To overcome these difficulties, the method of this problem solution based on the dual-regularization approach [5] has been developed for this problem also, and an algorithm of its numerical realization has been proposed [9]. It is important to note that a high enough accuracy is needed in the solution of this ill-posed problem. To achieve the necessary level of accuracy, multiple measurements have been averaged [7].

To avoid this difficulty, we propose to use the transformation of multifrequency data to that in time domain in the same way as in [10]. In such a synthesized pulse, measurement errors are shifted to large values of delay, so it is possible to use in the retrieval only the part of this pseudopulse that is free from large errors. Here we present the dual regularization method and the algorithm of its numerical realization for this modified inverse problem. Results of numerical simulation show that this new approach leads to the possibility to retrieve sharp profiles of inhomogeneities (at small differences from ideal meander structure) in conditions when the noise level in measurement data exceeds the informative part of signals.

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II. Theory

A. Inverse Problem Formulation

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

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

$i = 0, 2..., N/2$. 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 $f(z)$. 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*). However, the measurement errors can be comparable or even exceed the values of Δr_0. For example, to achieve the necessary level of accuracy multiple measurements have been averaged in [7] over 10 realizations. To avoid this difficulty, we propose here to use the transformation of multifrequency data to that in time domain in the same way as in [10]. For that, we consider the pseudopulse (inverse Fourier transform):

$$\Delta r_0(z_s) = \int_0^\infty \Delta r_0(\omega) \exp(i\omega z_s / c) d\omega \tag{4}$$

as a function of the parameter z_s of effective length of scattering. In such a synthesized pulse, measurement errors are shifted to large values of delay, so it is possible to use in the retrieval values of the pseudopulse in the interval $z_s \in [0, z_{s\max}]$ where it is free from errors.

B. Method of Dual Regularization

Then, this problem can be expressed as an equivalent problem of conditional minimization of the functional

$$I_0(f) \equiv \left\|f\right\|^2 \to \min,\ \Delta r[f](z_s) = \Delta r_0(z_s),\ f \in \mathrm{L}_2(0,d) \equiv \mathrm{D},\ z_s \in [0, z_{s\max}]. \tag{5}$$

The modified Lagrange functional of this problem is:

$$\begin{aligned} L_\mu(f,\lambda) = \| f \|^2 + \int_0^{z_{s\max}} [\lambda_1(z_s) \operatorname{Re}\left(\Delta r[f](z_s) - \Delta r_0(z_s)\right) + \lambda_2(z_s) \operatorname{Im}\left(\Delta r[f](z_s) - \Delta r_0(z_s)\right)] dz_x \\ + \mu\left\{\left(\int_0^{z_{s\max}} \left|\Delta r[f](z_s) - \Delta r_0(z_s)\right|^2 dz_s\right)^{1/2} + \int_0^{z_{s\max}} \left|\Delta r[f](z_s) - \Delta r_0(z_s)\right|^2 dz_s\right\}, \end{aligned} \tag{6}$$

where $\lambda = (\lambda_1, \lambda_2)$, $\mu > 0$. It is proved that the minimum of the modified Lagrange function $L_\mu(f, \lambda)$ over $f(z)$ in (6) is achieved at large enough values of μ at any $\lambda(z_s) = (\lambda_1(z_s), \lambda_2(z_s))$. The corresponding regularized modified dual problem that is the problem of minimization of the concave functional on the Hilbert space $L_2^2(z_{s1}, z_{s2}) = L_2(z_{s1}, z_{s2}) \times L_2(z_{s1}, z_{s2})$:

$$V_\mu^\alpha(\lambda) \equiv V_\mu(\lambda) - \alpha \|\lambda\|^2 \equiv \min_{f \in D} L_\mu(f, \lambda) - \alpha \|\lambda\|^2 \to \max, \lambda \in \Lambda_\mu \equiv \{\lambda \in L_2^2(z_{s1}, z_{s2}) : \|\lambda\| \le \mu\}. \quad (7)$$

where α is the Tikhonov's regularization parameter. The supergradient of this functional is expressed explicitly. Thus, the scheme of the dual regularization method consists of the gradient minimization of (6) at the simultaneous maximization of (7). The function $f(z)$ in the saddle point gives us the desired regularized solution. To realize all advantages 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 considered problem is so difficult that it is hardly possible to realize a universal algorithm for an arbitrary profile of inhomogeneity. 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. At the gradient minimization of the functional (6), the natural *a priory* constraint $0 \le f \le 1$ has been in use.

III. 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 λ=12.5÷14.5 nm at the elevation angle $\theta = 85^0$. 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 simulation are shown. The retrieval (Fig. 1a, where ε is given at λ=13.3 nm) has been obtained using "measurement data" with errors, which have been simulated by uncorrelated gauss-distributed random values $\delta r(\lambda)$ with *rms=0.036* (Fig. 1b), transformed to the pseudopulse (Fig. 1c).

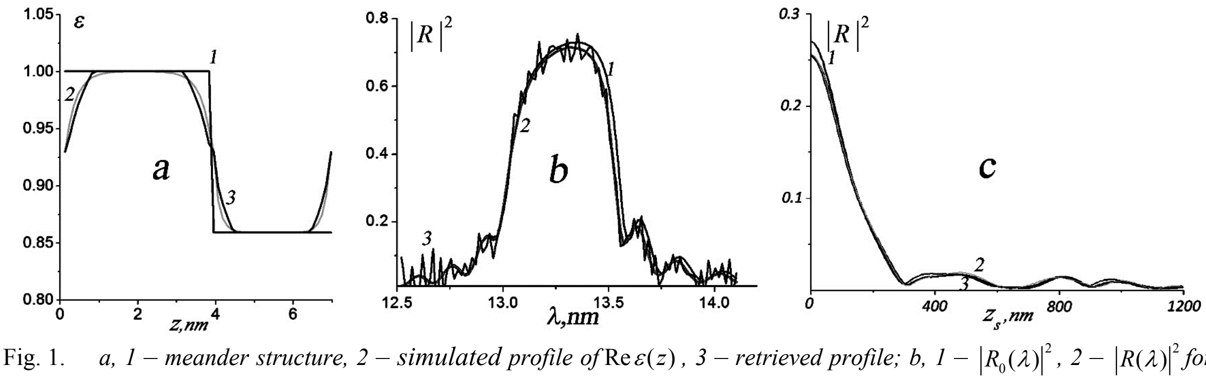

Fig. 1. *a, 1 – meander structure, 2 – simulated profile of* $\mathrm{Re}\,\varepsilon(z)$, *3 – retrieved profile; b, 1 –* $|R_0(\lambda)|^2$, *2 –* $|R(\lambda)|^2$ *for simulated profile, 3 –* $|R_m(\lambda)|^2$ *; c, corresponding synthesized pseudopulses: 1 –* $|R_0(z_s)|^2$, *2 –* $|R(z_s)|^2$, *3 –* $|R_m(z_s)|^2$.

One can see that "measurement" noise in Fig. 1b is mainly suppressed in the corresponding pseudopulse in Fig. 1c in the whole region of analysis – it is shifted to larger values of z_s. Just this fact made it possible to obtain good results of retrieval shown in Fig.1a. To demonstrate advantages of the data transformation more in detail, the informative part of the signal $|\Delta r| = \left||R|^2 - |R_0|^2\right|$ together with the noise distribution and their pseudopulse representations are shown in Fig. 2a and Fig. 2b, respectively.

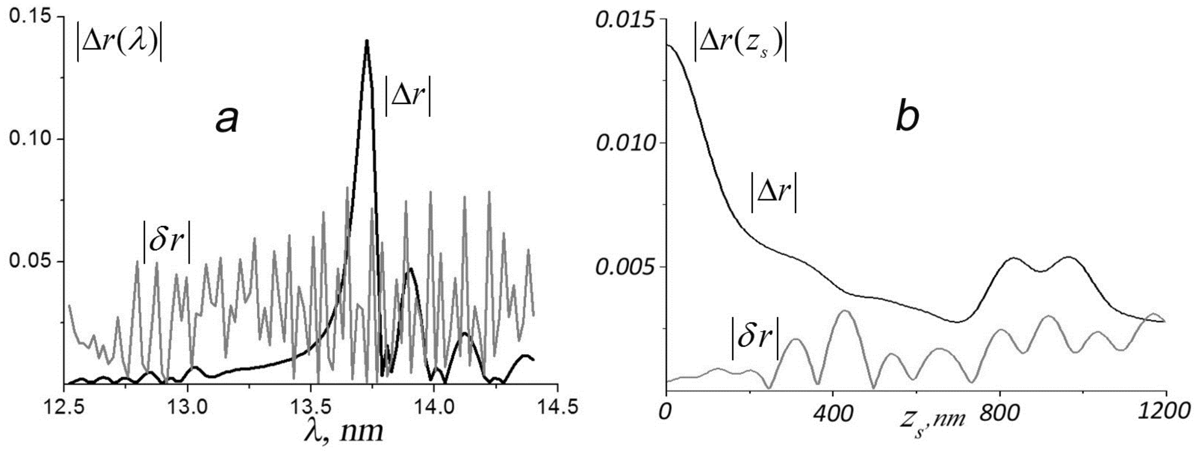

Fig. 2. *a, modulus of the informative part of signal* $|\Delta r(\lambda)| = \left||R(\lambda)|^2 - |R_0(\lambda)|^2\right|$ *for simulated profile and the random error* $|\delta r(\lambda)|$ *; b, corresponding synthesised pulses* $|\Delta r(z_s)| = \left||R(z_s)|^2 - |R_0(z_s)|^2\right|$, $|\delta r(z_s)|$ *vs. effective length of scattering.*

It easily seen in Fig. 2a that the noise mostly exceeds the measured spectrum of signal whereas, for their pseudopulse representations in Fig.2b, the noise appears much less than the desired signal.

VI. Conclusion

The numerical simulation of the proposed method of dual regularization in pseudopulse diagnostics of periodic structures demonstrates a good retrieval for profiles with sharp gradients of permittivity.

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