# **Reflectometry Sounding of Inhomogeneities in Periodic** Multilayer Structures

M. M. Barisheva, K. P. Gaikovich, P. K. Gaikovich, M. N. Polushkin, Yu. A. Vainer, S. Yu. Zuev Institute for Physics of Microstructures RAS, GSP-105, Nizhniy Novgorod, Russia Tel: +7(831)2581606, Fax: +7(831) 4385555, e-mail:Petek.RF@gmail.com

## ABSTRACT

In this paper, a reflectometry method of sounding of layers' parameters in periodic multilayered dielectric structures is proposed and applied to the study of X-ray optics structures. It is based on angular and spectral (multi-frequency) measurements of a studied structure. Angular measurements of the reflection coefficient are used to determine the period of a structure; the spectrum is in use to study the inhomogeneity of layers – the effective profile of dielectric permittivity related to the diffusion of material at the epitaxy and to the roughness of layers' interfaces. An integral equation has been obtained to solve this inverse scattering problem. An algorithm of the solution based on the Tikhonov's method of generalized discrepancy has been worked out, and the theory has been applied to study inhomogeneities of multilayer structures manufactured for the X-ray optics. **Keywords**: Reflectometry, multilayered periodic structures, permittivity profile

## **1. INTRODUCTION**

Multilayered periodical structures (MPS) are the basic elements of the modern X-ray optics. Since their invention in 1976 [1,2] they have been widely used as reflectors, polarisers and filters in the "soft" X-ray range, where crystals are irrelevant. MPS parameters were optimized for different purposes, but some deviations from a desired perfect meander structure appear at the synthesis. To examine MPS structures, X-ray scattering method examination in now widely in use: it has some obvious advantages: it is noncontact, nondestructive and fast in comparing to an electron microscopy or SIMS (secondary ion mass-spectrometry). One-dimensional structure defects can be described in the terms of permittivity profile by a mirror depth. The problem of the permittivity profile evaluation from the X-ray scattering data was discussed earlier for special cases. The theory represented in [3] can be interpreted as symmetrical meander structure with exponential transparent zones. In [4] authors propose the transparent zones linear model to estimate the asymmetry of the profile. In this paper we solve the inversion problem to obtain the permittivity profile in the most general case – without any presumptions about its shape or symmetry on the basis of the obtained integral equation.

# 2. THEORY

Let us consider a periodic multilayer (in z-direction) medium with the period  $d = d_1 + d_2$  with a complex permittivity profile  $\varepsilon(z) = \varepsilon'(z) + i\varepsilon''(z)$  expressed as

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

$$\varepsilon_{04}, z > Nd$$

where the profile of inhomogeneities  $\varepsilon_1(z) = \varepsilon_1(z+d)$  is also periodic. If the distribution of a probing electric field at  $\varepsilon_1 = 0$  is  $\mathbf{E}_0(\mathbf{r})$ , the total field  $\mathbf{E}(\mathbf{r})$  for a structure with inhomogeneities can be expressed as a sum of probing and scattered fields and obtained iteratively from the Fredholm equation of the 2-nd kind [5]

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{0}(\mathbf{r}) + \mathbf{E}_{1}(\mathbf{r}) = \mathbf{E}_{0}(\mathbf{r}) - \frac{i\omega}{4\pi} \int_{V} \ddot{\mathbf{G}}(\mathbf{r}', \mathbf{r}) \varepsilon_{1}(\mathbf{r}') \mathbf{E}(\mathbf{r}') d\mathbf{r}', \qquad (2)$$

beginning with the Born approximation

$$\mathbf{E}_{1}(\mathbf{r}) = -\frac{i\omega}{4\pi} \int_{V} \ddot{\mathbf{G}}(\mathbf{r}', \mathbf{r}) \varepsilon_{1}(\mathbf{r}') \mathbf{E}_{0}(\mathbf{r}') d\mathbf{r}' .$$
(3)

The Green tensor  $\mathbf{\tilde{G}}$  for a multilayer media can be obtained using the input impedance formalism [6,7]. The equation (3) can also be used to solve the inverse scattering problem [6]. In the considered case of the reflectometry of one-dimensional media, when plane waves are used as the probing field, the total field is also expressed as  $\mathbf{E}(\mathbf{r}) = \mathbf{E}(z)\exp(ik_x x + ik_y y)$ ; the problem is much simplified and reduced to the equation [8]:

$$\mathbf{E}_{1}(z) = -i\pi\omega \int_{z'} \varepsilon_{1}(z') \ddot{\mathbf{g}}(z', z) \mathbf{E}_{0}(z') dz', \qquad (4)$$

In the case of X-ray optics, further simplifications are possible. First of all, permittivity perturbations are so small that the Born approximation is satisfied with a high accuracy. Hence, we can obtain from (4) a quite simple equation for the perturbation of the reflection coefficient  $R_1$ . It depends on the viewing angle and frequency and can be written in a compact form as:

$$R_{1}(\theta,\omega) = \int_{z'} \varepsilon_{1}(z')g(\theta,\omega,z')dz', \qquad (5)$$

where  $g(\theta, \omega, z')$  includes contributions of Green functions for TE and TH polarizations. Then, it is possible to use the periodicity property of  $\varepsilon_1(z')$  to obtain the desired expression for the scattering of the considered structure with periodic one-dimensional inhomogeneities:

$$R_1(\theta,\omega) = \int_d \varepsilon_1(z) \sum_{i=1}^{\frac{N-1}{2}} g[\theta,\omega,z+(i-1)]dz, \qquad (6)$$

Considering (6) as the integral equation, we can solve the corresponding inverse problem of scattering to retrieve the profile  $\mathcal{E}_1(z)$  over the period of a multilayer structure using data of angular or frequency measurements.

However, in most cases the power reflection coefficient is measured:

$$|\mathbf{R}|^{2} = |\mathbf{R}_{0}|^{2} + 2\operatorname{Re}(\mathbf{R}_{0}^{*}\mathbf{R}_{1}) + |\mathbf{R}_{1}|^{2}.$$
(7)

The reflection coefficient of the unperturbed structure  $|R_0|^2$  (the first term in the right-hand side of (7)) can be calculated, if we know the geometry  $(d_1, d_2, N)$  and dielectric parameters of layers; two last terms determine the contribution of scattering. So, combining measured and calculated data, we can use  $\Delta r(\theta, \omega) = |R|^2 - |R_0|^2$ , obtain the expression

$$\Delta r(\theta,\omega) = \int_{d} 2\operatorname{Re}\left\{R_{0}^{*}\varepsilon_{1}(z)\sum_{i=1}^{\frac{N-1}{2}}g[\theta,\omega,z+(i-1)]\right\}dz + \left|R_{1}[\varepsilon_{1}(z)]\right|^{2}.$$
(8)

Because  $\varepsilon_1(z)$  is related to mutual penetration of two component, it is possible to represent it as  $\varepsilon_1(z) = f(z)(\varepsilon_{03} - \varepsilon_{02})$ , where the real profile f(z) (-1 < f(z) < 1) determines the complex permittivity perturbations. Then, this expression can be reduced to the integral equation that can be solved iteratively:

$$\Delta r(\theta, \omega) = \int_{d} f^{(n)}(z) \operatorname{Re} \left\{ 2R_{0}^{*}(\varepsilon_{03} - \varepsilon_{02}) \sum_{i=1}^{\frac{N-1}{2}} g[\theta, \omega, z + (i-1)] \right\} dz + \left| R_{1}(f^{n-1}(z)) \right|^{2}.$$
(9)

Denoting  $\Delta r^i(\theta, \omega) = |R|^2 - |R_0|^2 - |R_1(\varepsilon_1^{i-1}(z))|^2$ , the integral equation of the inverse scattering problem can be written in a compact form as:

$$\Delta r^{(n)}(\theta,\omega,f^{(n-1)}) = \int_{0}^{d} f^{(n)}(z) K(\theta,\omega,z) dz \,. \tag{10}$$

At each step of the iteration, the equation (10) is a Fredholm integral equation of the 1-st kind. To solve this ill-posed problem, we use the Tikhonov's method of generalized discrepancy [9].

#### **3. EXPERIMENTAL STUDY**

The proposed method has been applied to the study of the permittivity perturbations in the multilayer X-ray mirrors. It is well-known that depths  $d_1, d_2$  of layers can be determined for these periodic structures from angular reflectometry measurements at a short enough wavelength using the best fit. In Fig.1 it is possible to see an example of measurements of  $|R(\theta)|^2$  at the wavelength  $\lambda = 0.154$  nm and the result of the rms fitting for the periodic Mo-Si 50-layer structure.



Figure 1. (1)Angular measurements of the reflection coefficient; (2)rms fitting.

The layer's depths determined from this fitting are  $d_1 = 3.79$  nm;  $d_2 = 3.30$  nm.

Then, the permittivity inhomogeneities over the period of this structure have been studied using multifrequency measurements at longer waves in the range  $\lambda = 12.5 - 14.5$  nm at the  $\theta = 80^{\circ}$ . The main condition for a successful solution of the inverse scattering problem (i.e. of the equation (10)) is the sensitivity of measurements to the profile variations. In the Fig.2 one can see that in the chosen spectral range the kernel of (10) has a high depth-frequency variability that ensures the proper sensitivity.



Figure 2. The depth-frequency distribution  $K(\omega, z)$  of the kernel in (10).

In Fig.3a results of spectral measurements of  $|R(\omega)|^2$  are shown along with the distribution of  $|R_0(\omega)|^2$ , calculated on the base of angular measurements and the distribution  $|R(\omega)|^2 = |R_0|^2 + |R_1(f^{(2)})|^2$  obtained from

the solution of (10) at the second step of iteration. In Fig.3b one can see results of the solution of the inverse scattering problem – the retrieved profile  $\varepsilon(z)-1$  in the studied periodic structure.



(b), retrieved profiles of  $\operatorname{Re} \varepsilon(z) - 1$  and  $\operatorname{Im} \varepsilon(z)$ .

Obtained profiles of permittivity are obviously asymmetric with different depths of transition regions that give important information about studied structures.

# 4. CONCLUSIONS

A reflectometry method has been worked out to solve the inverse scattering problem in periodic multilayer structures and applied to the study permittivity profile in X-ray mirrors.

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