Numerical simulation of gliding reflection of X-ray beam from rough surface

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Abstract

A new method for investigation of X-ray beam propagation in a rough narrow dielectrical waveguide is proposed on the basis of the numerical integration of the quasioptical equation. In calculations a model rough surface is used with the given distribution of heights of roughness and given correlation properties of the surface. The method is free from the limitations such as infiniteness of the surface length and plane wave approximation which are necessary for application of Andronov-Leontovich method. Our method can be applied to any surface with given nonhomogeneity and distribution of transitional layer.

Key words: numerical simulation, X-ray radiation, rough surface
In the middle of 1970-s the experiments on channelization of soft X-rays \[1\] and middle range X-rays \[2\] in glass tubes and also for filtering of hard part of X-ray radiation in bent tubes bundles \[3\]. The workability of such systems was demonstrated for transport of X-ray radiation. Later the interest to this manner of X-ray steering was connected with the suggestion to use the samples of many specially bent tubes for geometrical focusing and concentrating of X-ray beam \[4\]. The experiments were performed for transmission of X-ray beam through “gap-less collimator” - micron gap between two tightly pressed together glass plates \[5, 6\]. The revival of interest to localizing of X-rays in thin glass capillaries of changing diameter in the condition of total external reflection at grazing incidence on smooth surface was connected with the attempts of microfocusing in a narrowing tube \[7\] (till 7\(\mu\)m) or in a narrowing polycapillary system \[8\], consisting of a great number of melted-in together thin glass tubes forming one hexahedral block. The problems of the structure of the focus of such system deals with the work \[9\].

The channalisation of X-ray radiation in hollow glass tubes is possible due to the effect of total external reflection \[10\]. The dielectric permeability of substance for electro-magnetic radiation with the energy higher than binding energy of electrons in atoms can be approximately written with the use of plasma frequency \(\omega_p\) \[4\]

\[
\varepsilon(\omega) = 1 - (\omega_p/\omega)^2.
\]

Because in X-ray energy range \(\varepsilon(\omega) < 1\) and optical density of glass is smaller than the vacuum (or air) optical density the effect of total external reflection takes place when the rays come from outside and for this reason is called total external reflection (TER).

When X-ray radiation comes on sufficiently smooth surface in the conditions of TER the radiation penetrates only at small depth of the order of 60\(\AA\), that maintains the effective reflection and channalisation of radiation in hollow glass tubes.

Besides of the absorption the effectiveness of reflection depends strongly on the scattering of radiation on roughness of the surface. The most of the results on the influence of roughness on the reflection of X-ray radiation from surfaces were obtained in the approximation of Andronov and Leontovich \[11\]. The review of the results can be found in \[12\]. The approximation is based on the suggestion that the initial wave coming on the surface is a plane wave and the scattered wave can be found for small perturbations of the boundary between two media. That is why the investigation of scattering of wave coming on absorbing surface at small
angles is interesting because in this case the Andronov and Leontovich approximation apparently can not be applied any longer.

1 The derivation of master equation.

Maxwell equations are \[13\]

\[
\begin{align*}
\text{rot} \mathbf{H} &= \frac{\varepsilon}{c} \frac{\partial \mathbf{E}}{\partial t} + \frac{4\pi \sigma}{c} \mathbf{E}, \\
\text{rot} \mathbf{E} &= -\frac{\mu}{c} \frac{\partial \mathbf{H}}{\partial t}, \\
\text{div} \mathbf{E} &= 0, \\
\text{div} \mathbf{H} &= 0.
\end{align*}
\]

We can exclude the vector \( \mathbf{H} \) by applying to the second equation the operation \( \text{rot} \text{rot} \mathbf{E} = \text{grad} \text{div} \mathbf{E} - \Delta \mathbf{E} \).

With account of the third Maxwell equation we get wave equation:

\[
\Delta \mathbf{E} - \frac{\epsilon \mu}{c} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{4\pi \sigma \mu}{c^2} \frac{\partial \mathbf{E}}{\partial t} = 0. \tag{1}
\]

Furthermore, represent the vector of the electric field in the form

\[
\mathbf{E} = \frac{\mathbf{e}}{2} A(x, y, z) \exp[i(\omega t - k z)] + ..
\]

\( k = \sqrt{\epsilon_0 \frac{\mu}{\varepsilon}} \). (In this case \( \epsilon_0 \) is dielectrical permeability of air, \( \varepsilon \)- dielectrical permeability of glass.) It can be shown that the speed of changing of the amplitude \( A(z, x, y) \) in the beam is different for the transversal coordinates \( x, y \) and longitudinal coordinate \( z \) \[13\]. The evolution along the direction \( z \) is much slower than along transversal coordinates. Thus after substituting of (2) into wave equation (1) we can neglect terms \( \frac{\partial^2 A}{\partial z^2} \) in comparison with \( k(\partial A/\partial z) \) and \( \partial^2 A/\partial x^2 \), resulting to so called parabolic equation of quazioptics:

\[
2ik \frac{\partial A}{\partial z} = \Delta_{\perp} A + k^2 \frac{\delta \epsilon}{\epsilon_0} A \tag{3}
\]

where the difference between the dielectrical permeabilities \( \delta \epsilon = \epsilon - \epsilon_1 \) depends on coordinates and includes imaginary part corresponding to absorption in the substance.
2 The method of simulation of rough surface.

Under the total external reflection at grazing incidence of X-ray beam the most important is scattering within the plane of incidence because the scattering withing the plane of the interface is small \[12\]. First of all it is due to the fact that the wavelength of the radiation is much smaller than the characteristic scale of inhomogeneities. That is why for simulation of scattering of X-rays at TER conditions it is enough to account for only scattering in the plane of incidence within 2-dimensional model. In this case the value \( \delta \epsilon \) in the right side of equation (3) becomes the function of coordinates \( z \) and \( x \):

\[
\delta \epsilon(x, z) = \begin{cases} 
0, & x > \xi(z) \\
\epsilon - \epsilon_0, & x < \xi(z)
\end{cases},
\]

where the function \( \xi(z) \) is the height of the rough surface profile and can be regarded as a random value (see Fig.1()).

Stationary random value on the interval \( (0, Z) \) can be expanded in the Fourier series \[14\] :

\[
\xi(z) = \sum_{k=1}^{\infty} V_k \cos \omega_k z + U_k \sin \omega_k z, \quad 0 \leq z \leq Z,
\]

where \( V_k, U_k \) are random amplitudes of the harmonics \( \omega_k = k \omega_1 \),

\[
\omega_1 = \frac{2\pi}{Z_1}
\]

\( Z_1 \) is maximum spacious period of random sequence. In the discrete representation

\[
\xi(n) = \sum_{k=0}^{m} V_k \cos \frac{k \pi n}{N} + U_k \sin \frac{k \pi n}{N}, \quad n = 1, N;
\]

where \( V_k \) and \( U_k \) uncorrelated random numbers with the dispersion \( \sigma_k^2 \) and zero mean value. The dispersion of the harmonics is

\[
\sigma_k^2 = \frac{2}{\pi} \int_0^{\infty} R(\xi) \cos(k \omega_1 \xi) d\xi,
\]

where \( R(\xi) \) is correlation function of the random value \( \xi(z) \). For normal random processes the amplitudes \( V_k \) and \( U_k \) must have normal distribution \[14\]. The expression for \( \xi(n) \) can be also represented as
\[ \xi(n) = \sum_{k=0}^{m} E_k \cos\left( \frac{k\pi n}{N} + \alpha_k \right), \]  \hspace{1cm} (5)

where \( E_k \) is random coefficient with Rayleigh distribution with the parameter \( \sigma \) equal to \( \sigma_k \), where \( \alpha_k \) is random phase of the harmonics with the uniform distribution on the interval \( (0, 2\pi) \).

For choosing of the number of harmonics \( m \) a relationship can be used

\[ 1 - \frac{1}{R(0)} \sum_{k=0}^{m} \sigma_k^2 \ll 1, \]

so the sum of dispersions \( \sigma_k^2 \) must be equal to the dispersion of the simulated process.

### 3 Numerical results and discussions.

The numerical method for solving of the equation (1) was used earlier for study of motion of channeled electrons in single crystals [15] and reflection of positrons from slanting cut single crystals [16]. The method implies step by step calculation of the amplitude of the X-ray wave \( A(x, z) \) along the surface of reflection starting from its initial value at \( z=0 \).

For simulation of a rough surface the code was constructed calculating random sequence of numbers \( \xi(n) \) in accordance with representation (5). With the given correlation function by relationship (4) the amplitudes \( E_k \) of spectral components were determined. For simulation of random phase \( \alpha_k \) random numbers generators were used. Fragments of random surface \( \xi(n) \) is presented on Fig. 1(a). With account of several realisation of numerical process with different number of points correlation functions were calculated again along with probability density distribution. On Fig. 1(b) the comparison of given correlation function (curve 1) and correlation functions calculated with realisation of \( n=1000 \) points (curve 2) and \( n=10\,000 \) points (curve 3 that nearly coincides with 1). It is obvious that with the increase of \( n \) correlation function of the process \( \xi(n) \) approaches the given function. It was also shown that the distribution of the probability density for random process \( \xi(n) \) approaches Gaussian distribution when the number of points in the realisation increases (Fig.1(c)).
So we can affirm that the created code simulates random surface with the given statistical characteristics and Gaussian probability density distribution.

The calculations were made for the radiation with the energy 10 keV and for interaction with rough glass surface. The width of the correlation function was chosen 5\( \mu \)m. The angle of total external reflection is \( \varphi_c = 3 \cdot 10^{-3} \text{rad} \).

When the angle of incidence of X-ray wave is not zero the surface can be regarded as infinite and incident wave as a plane wave. On Fig. 2 the distribution of the intensity of the radiation along the coordinate \( x \) (the axis \( x \) is perpendicular to the surface) for reflection from smooth surface for the angle of incidence \( \varphi = 10^{-3} \text{rad} \). The range \( 0 < x < 2100 \text{Å} \) corresponds to the substance layer. The oscillations of the intensity are caused by the interference of incident and mirror reflected waves. At some distance from the surface that is defined by numerical scheme parameters the amplitude was smoothly truncated that is dependent on the use of the Fourier transformation on the \( x \) coordinate for solving the equation (3) (see Fig.2).

With the increasing of roughness amplitude the angular spectrum of the reflected beam the mirror reflected beam decreases and at the same time numerous random maxima arise so that clear interference diffraction picture disappears near the surface. Simple estimate for roughness tolerance of total external reflection observation was given in [17] \( h \leq \lambda_0/8\varphi_0 \),

where \( \lambda_0 \) is the radiation wavelength. As a clear illustration of inverse dependence of tolerable roughness amplitude on the incidence angle can be used angular spectra of reflection shown on Fig. 3. The spectra were calculated for angles \( 0.5 \cdot 10^{-3} \text{rad. (a)}, 10^{-3} \text{rad. (b)}, 2 \cdot 10^{-3} \text{rad. (c)} \) for the same roughness amplitudes 200 Å (here and further the mean squared roughness amplitude is used). In the first case the influence of roughness on the spectrum is small but in the last case the mirror reflected peak can not be observed in practice.

The calculations of the distribution of the intensity of radiation near the smooth reflecting surface can show the depth of penetration of X-rays into the surface under the conditions of TER as a function of the incidence angle and for \( \varphi = 10^{-3} \text{rad} \), it is 60 Å, for \( \varphi = 10^{-4} \text{rad. - 10 Å} \). For reflection from rough surfaces the depth of penetration (counted from the mean value of the roughness) is approximately equal to the mean squared amplitude of roughness.
With the created complex of codes calculations were performed for transmission of X-ray radiation in a 2-dimentional rough capillary for zero and near to zero entrance angles. Transversal dimensions of capillaries were chosen $1 - 2\mu m$, that caused diffractional spreading of the plane wave to the values $0.5 \cdot 10^{-4} - 10^{-4} rad$. The length was chosen as $1 - 2 cm$.

On Fig.4 the dependence of integral intensity (over the transversal dimension of the capillary) on the distance from the entrance to the capillary. The angle of incidence $\varphi_0 = 0$, the width of the capillary is $2\mu m$, the roughness is $1200 \AA$. Abrupt falling of the intensity of the radiation in the input of the capillary is connected with the absorption of the radiation coming on glass butt-ends and transmitting within the substance. This part of the radiation can be regarded as fully absorbed at the distance $z \leq 1000 \mu m$ from the input of the capillary. The analysis of the distribution of losses along the capillary length for $z \geq 1000 \mu m$ reveals its considerable dependence on the distance from the capillary input. The deeper radiation penetrates the capillary the smaller loss normalized to the length unit is that is apparently related to consequent decay of modes the most strongly penetrating into the substance.

The losses of radiation in the capillary are the greater the the greater capillary wall roughness is and the bigger the angle of incidence of the wave into the capillary is. The partial dependence of losses of the radiation (size for zero incidence angle and angle value $10^{-4} \text{ rad}$ is shown on Fig.5. The losses were calculated on the range $0.25 cm \leq z \leq 1 cm$ from the capillary input. It is worth noting that losses are not zero even for the capillary with smooth walls.

The dependence of losses of radiation in capillaries of various widths with wall roughness $800 \AA$ and $400 \AA$ and also without roughness for zero incidence angle are shown on Fig.6. The increase of losses when the width of the capillary $\Delta x$ is decreased can be accounted for by the broadening of the plane wave incident on the input of the capillary $\Delta \varphi = \lambda_0 / \Delta x$.

On Fig.7 radiation angular spectra are shown for capillaries with the length $1 cm$ of various widths with smooth and rough walls. The calculations were made for zero incidence angle. The decrease of the square under the spectral peak along with the increase of roughness can be accounted for by higher absorption of the radiation but the shape and the width of the spectral peak practically does not depend on the roughness size.
4 Conclusion.

So the created code can simulate interaction of X-rays with rough surface (including zero gliding angle) without supposition of infinite plane wave but with direct account of given surface relief. That is the advantage of the approach over analytical methods (including Andronov-Leontovich approximation). In comparison with numerical methods using geometrical optics the proposed method takes into account the wave nature of the radiation (diffraction).

The obtained results enable also to give new interpretation of the experiments with "gapless collimator" published in 1981-1984 [5, 6]. According to the data of angular distance between interference peaks in transmitted beam with account of diffraction the gap width is 10\(\mu\text{m}\) but not 1\(\mu\text{m}\) as it follows from [6] without account for diffraction. In this case different number of transversal modes is excited depending on the tilt angle of input beam. On the other hand if in glass plates unpolished transversal band is left the independence of output beam on the input beam tilt can be explained due to strong absorption of higher transversal modes along with retaining of lowest symmetric mode (see Fig.7).

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Fig. 1a. Fragment of calculated surface with account of equation (5).
Fig. 1b. 1 - given initially correlation function;
2 (dashed) - correlation function calculated with realization of random sequence (n) with 1000 points;
3 - correlation function for sequence with 10000 points.
Fig. 1c. 1 - gaussian distribution with given parameters,  
2 - distribution of density probability calculated with realization  
of random sequence (n) with 10000 points.
Fig. 2. Distribution of intensity of X-ray radiation in the vicinity of smooth reflective surface in the conditions of the Total External Reflection at the angle of incidence on the surface $\varphi_0 = 10^{-3}$ rad. Axis $x$ is perpendicular to the surface. Reflecting layer of the substance is within $0 < x < 2100\text{Å}$; reflecting surface is marked with dash line.
Fig.3. Angular spectrum of reflection of X-ray radiation from the surface with roughness amplitude 200Å for incidence angle to the surface $\varphi_0 = 0.5 \cdot 10^{-3}$ rad.
Fig. 3bc. The same as Fig. 3 for $\varphi_0 = 10^{-3} \, rad$ (b) and $\varphi_0 = 2 \cdot 10^{-3} \, rad$ (c).
Fig.4. Dependence of integral over the width of the capillary $x = 2 \, \mu m$ intensity of radiation on the depth of capillary $Z$. Angle of incidence of plane wave to the input of the capillary $\varphi_0 = 0$, wall roughness is 1200Å.
Fig. 5. Dependence of losses of radiation (%) calculated at the distance $0.25\text{cm} < Z < 1.0\text{cm}$ from the input of the capillary on the averaged amplitude of roughness at the capillary walls $(\sigma_{\xi}^2)^{1/2}$ - mean squared deviation for roughness $\xi$. Angles of incidence of X-ray beams to the input of capillary $\varphi_0 = 10^{-4} \text{ rad}\,(1) \varphi_0 = 0 \text{ rad}\,(2)$. The capillary width is $2\mu m$. 
Fig. 6. Dependence of losses of radiation (%) calculated within the range $0.25 < z < 1.0\text{cm}$ from the input of the capillary. Angle of incidence $\varphi_0 = 0$. Roughness of capillaries is $800\AA (1), 400\AA (2)$, smooth walls (3).
Fig. 7a. Angular spectra of the radiation at the output of capillaries with length 1cm for smooth capillaries (solid lines) and with rough capillaries 400Å (dashed lines). Width of capillaries is 0.5µm. Angle of incidence is \( \varphi_0 = 0 \).
Fig. 7b. The same as Fig. 7a but for roughness 800 Å and width of capillaries 1 µm.
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