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Influence of the Spatial Coherence of X-ray Radiation on Mirror Reflection from Multilayered Mirrors

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Abstract—The influence of the degrees of spatial coherence of random modulated X-ray radiation on the intensity of the diffractive reflection of such radiation from a multilayered mirror, and on the spatial coherence function of the reflected field (depending on the statistical characteristics of the incident radiation and the parameters of the multilayered periodic structure), is considered.

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INTRODUCTION

Diffractive reflection of X-ray and synchrotron radiation from crystals and multilayered periodic structures (MSes) is widely used in the monochromatization and collimation of radiation. It is known that electromagnetic fields irradiated by nonlaser radiation sources are random (Gaussian, as a rule) [1]. The coherency properties of X-ray radiation considerably influence both the statistical properties of this radiation as it propagates in free space [2, 3] and the formation of phase-contrast [4–7] and coherent diffractive [8–12] images of various crystal, amorphous, and medicobiological objects. It is therefore important to determine the length of spatial coherence (LSC) and the sizes of synchrotron radiation sources [7, 10, 13–15] and X-ray laser pulses on free electrons [11, 12].

This paper studies the influence of the degree of spatial coherence of X-ray radiation falling on a multilayered structure on the spatial coherence function (SCF) of the radiation after its reflection from the MS. It is also shown that even such a simple optical element as a slit leads to a quite substantial change in the transmitted radiation's SCF, i.e., to the appearance of a local statistical irregularity in the cross section of the transmitted beam.

REFLECTION OF A RANDOM X-RAY BEAM

Let us study the reflection from an MS of partially coherent (correlated), stationary-in-time X-ray radiation with a field represented as

$$E_0(x,z) = A_0(x,z)\exp(i\mathbf{k}_0\mathbf{r}), \tag{1}$$

where $\mathbf{k}_0$ is the medium (central) wave vector with value $k_0 = |\mathbf{k}_0| = 2\pi/\lambda$, λ is the wavelength; $A_0(x, z)$ is in the general case a random complex field amplitude; axis x is directed along the surface of MS; and axis z is directed into the depths of the medium normal to the surface. Here, $k_{0x} = k_0\cos\theta$, $k_{0z} = k_0\gamma_0$, where $\gamma_0 = \sin\theta$ and θ is the arbitrary angle of the beam incidence (1) relative to MS surface.

Let us represent random field (1) on the surface of the MS $z = 0$ as a Fourier expansion by plane waves:

$$E_0(x) = E_0(x,0) = \int_{-\infty}^{\infty} E_0(k_x)\exp(ik_x x)dk_x, \tag{2}$$

where

$$E_0(k_x) = (2\pi)^{-1}\int_{-\infty}^{\infty} E_0(x)\exp(-ik_x x)dx. \tag{3}$$

Let us substitute field (1) into (3) and introduce variable $q = k_x - k_{0x}$. If the characteristic cross section dimension of the beam is $r_0 \gg \lambda$, spectral amplitude

$$E_0(k_x) = A_0(q) = (2\pi)^{-1}\int_{-\infty}^{\infty} A_0(x)\exp(-iqx)dx \tag{4}$$

differs considerably from zero only at $|q| \ll k_{0x}$ (the quasi-optical approach in [16]) and, like $A_0(x)$, is a random function of argument q. Field (1) can be represented as the set of plane waves $A_0(q)\exp(i\mathbf{kr})$ falling on MS, where $k_x = k_{0x} + q$ and $k_z = (k_0^2 - k_x^2)^{1/2}$. If $R(k_x)$ is the amplitude reflection ratio, each spectral component reflects with amplitude $R(k_{0x} + q)A_0(q)$ and wave vector $(k_x, -k_z)$. Let us now assume that at $\xi \ll 1$, expansion $(1 + \xi)^{1/2} \approx 1 + \xi/2 - \xi^2/8$ is true. The z-projection is then $k_z \approx k_{0z} - q\cot\theta - q^2/(2k_0\gamma_0^3)$. Finally, we obtain the following expression for the reflected wave's field at arbitrary point $(x, z < 0)$: $E_R(x, z) = A_R(x, z;\theta)\exp(i\mathbf{k}_R\mathbf{r})$, where $\mathbf{k}_R = (k_{0x}, -k_{0z})$ and random amplitude A_R takes the form

$$A_R(x,z;\theta) = \int_{-\infty}^{\infty} R(k_{0x} + q)A_0(q)\exp(i\Phi_1 + i\Phi_2)dq. \tag{5}$$

Here, phase $\Phi_1(x, z, q) = (x - |z|\cot\theta)q$ describes an out-of-plane shear of the reflected beam along axis x, while phase $\Phi_2(z, q) = q^2z/(2k_0\gamma_0^3)$, quadratic by q, describes diffractive beam spreading as distance $L = |z|/\gamma_0$ from the MS increases along the direction of reflection $\mathbf{k}_R$.

The statistical properties of the incident field are described by transverse SCF (or correlated function) $\Gamma_0(x_1, x_2)$ and normalized per unit by coherence degree $\gamma_0(x_1, x_2)$ [1]:

$$\Gamma_0(x_1, x_2) = \langle A_0(x_1)A_0^*(x_2)\rangle, \qquad (6)$$

$$\gamma_0(x_1, x_2) = |\Gamma_0(x_1, x_2)|/[I_0(x_1)I_0(x_2)]^{1/2}, \qquad (7)$$

where $I_0(x) = \langle|A_0(x)|^2\rangle = \Gamma_0(x, x)$ is the field intensity at point x; chevrons denote the averaging within the period of time, which considerably exceeds the characteristic time of field fluctuation. For fully coherent fields, function $\gamma_0(x_1, x_2) = 1$ at any values $x_1 \neq x_2$. However, in the general case for partially coherent fields, $0 < \gamma_0(x_1, x_2) < 1$.

Using (2)–(4), the total energy W_0 coursing through the cross section of the incident beam can be represented as

$$W_0 = \int_{-\infty}^{\infty} I_0(x)dx = 2\pi\int_{-\infty}^{\infty}\Gamma_0(q)dq, \qquad (8)$$

where $\Gamma_0(q) = \langle|A_0(q)|^2\rangle$ is the angular spectrum (spectral density) of a random field. It follows from ratios (4) and (6) that this is defined by inverse SCF Fourie transformation $\Gamma_0(x_1, x_2)$ (6):

$$\Gamma_0(q) = (2\pi)^{-2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Gamma_0(x_1,x_2)\exp[-iq(x_1 - x_2)]dx_1dx_2. \qquad (9)$$

Let us now proceed to a discussion of the influence of the statistical characteristics (6) of radiation incident upon the SCF of reflected radiation $\Gamma_R(x_1, x_2; z) = \langle A_R(x_1, z; \theta)A_R^*(x_2, z; \theta)\rangle$ in arbitrary plane z on the intensity profile of reflected beam $I_R(x, z; \theta) = \Gamma_R(x, x; z)$ at fixed angle θ, and on reflection curve $P_R(\theta)$. Taking into consideration ratio (5), the SCF of reflected field will have the following integral form:

$$\Gamma_R(x_1, x_2; z)$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} R(k_{0x} + q_1)R^*(k_{0x} + q_2)\Gamma_0(q_1, q_2) \qquad (10)$$

$$\times \exp[i\xi_1q_1 - i\xi_2q_2 + i(q_1^2 - q_2^2)z/(2k_0\gamma_0^3)]dq_1dq_2,$$

where $\xi_{1,2} = x_{1,2} - |z|\cot\theta$,

$$\Gamma_0(q_1, q_2)$$

$$= \langle A_0(q_1)A_0^*(q_2)\rangle \qquad (11)$$

$$= (2\pi)^{-2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Gamma_0(x_1,x_2)\exp(-iq_1x_1 + iq_2x_2)dx_1dx_2.$$

It is easy to show from ratio (10) that total energy $W_R(\theta)$ coursing through the cross section of the reflected beam is independent of distance z; this signifies conservation of energy as the beam propagates from the MS to the detector:

$$W_R(\theta) = \int_{-\infty}^{\infty} I_R(x,z;\theta)dx = 2\pi\int_{-\infty}^{\infty}|R(k_{0x} + q)|^2\Gamma_0(q)dq. \qquad (12)$$

The curve of reflection, defined as $P_R(\theta) = W_R(\theta)/W_0$, is proportional to convolution (12) of curve of reflection $|R(k_{0x} + q)|^2$, calculated for a coherent plane wave, with function of spectral density $\Gamma_0(q)$. Angular spectrum $\Gamma_0(q)$ of the incident radiation can be interpreted as an instrument function, as is often done when comparing theory to experiment.

It should be emphasized that the statistical characteristics of incident radiation are integrally incorporated into curve of reflection (12) and are defined mainly by width Δq_0 of function $\Gamma_0(q)$. At the same time, width Δq_0 depends on such parameters as the size of the incident beam, the regular field phase, the LSC, and the shape of the SCF (see (21) below and [3]). One and the same value Δq_0 can be found for different sets of these parameters, which is why they cannot be defined from the measured curve of reflection. Moreover, the curve of reflection does not at all depend on the statistical characteristics of the reflected beam. In contrast to this, SCF (10) and the profile of the intensity of reflected beam $I_R(x, z; \theta)$ are more sensitive to the parameters listed above. This can be seen clearly, e.g., upon registration of the phase-contrast images of objects placed in the reflected beam [3, 7, 9].

RESULTS AND DISCUSSION

General ratios (9)–(12) are significantly simplified in the widely used simple special case, in which the incident radiation is random plane wave $E_0(x') = A_0(x')\exp(ik_0z')$ whose intensity $I_0 = \langle|A_0(x')|^2\rangle$ does not depend on coordinate $x' = x\gamma_0$ in the wave cross section. Since such a wave is statistically homogeneous, its SCF $\Gamma_0(\rho) = \langle A_0(x)A_0^*(x + \rho)\rangle$ must depend only on difference ρ between the points. The spectral amplitudes $A_0(q)$ must therefore be δ-correlated [1], i.e., $\Gamma_0(q, q') = \Gamma_0(q)\delta(q - q')$. SCF $\Gamma_0(\rho)$ (6) and spectral density $\Gamma_0(q)$ (9) of such a wave will then take the following form:

$$\Gamma_0(\rho) = \int_{-\infty}^{\infty}\Gamma_0(q)\exp(-iq\rho)dq, \qquad (13)$$

$$\Gamma_0(q) = (2\pi)^{-1}\int_{-\infty}^{\infty}\Gamma_0(\rho)\exp(iq\rho)d\rho. \quad (14)$$

Substituing $\Gamma_0(q, q')$ into (10), we get the following ratio for the SCF of the reflected random plane wave, which is of course independent of x and z:

$$\Gamma_R(\rho;\theta) = \int_{-\infty}^{\infty}|R(k_{0x}+q)|^2\Gamma_0(q)\exp(-iq\rho)dq. \quad (15)$$

If, e.g., the SCF of the incident wave is (13) in plane $z = 0$ has the form of a Gaussian function (i.e., $\Gamma_0(\rho) = \exp[-(\rho\gamma_0/\rho_0)^2]$, where ρ_0 is the spatial coherence length), the spectral density has a Gaussian form as well:

$$\Gamma_0(q) = (1/\Delta q_0\pi^{1/2})\exp[-(q/\Delta q_0)^2], \quad (16)$$

where $\Delta q_0 = 2\gamma_0/\rho_0$ is the width of the angular spectrum. Here and below, the well-known tabulated ("optical") integral is used in our calculations:

$$\int_{-\infty}^{\infty}\exp(iax+ibx^2)dx = (i\pi/b)^{1/2}\exp(-ia^2/4b), \quad (17)$$

where a and b are any complex values.

New now let a random Gaussian beam fall on the MS with amplitude

$$A_0(x') = \exp[-(x'/r_0)^2(1-i\alpha_0) + i\varphi(x')], \quad (18)$$

where r_0 is the transverse beam size; x' is the transverse coordinate; α_0 is the parameter of the regular (quadratic by x') phase describing in approximation the quazioptically parabolic bend of a wave surface; and $\varphi(x')$ is a random phase. We also imagine that the degree of coherence, which is the local statistical characteristic of the incident field for defined points x_1' and x_2' and depends only on the difference $\rho' = x_2' - x_1'$ (i.e., describes a type of locally homogeneous random fields), has a Gaussian form as well:

$$\gamma_0(x_1', x_2') = \langle\exp[i\varphi(x_1') - i\varphi(x_2')]\rangle = \exp[-(\rho'/\rho_0)^2], \quad (19)$$

where ρ_0 is the LSC of radiation of incident beam. We substitute (18) and (19) into (11) and obtain the following analytical expression for correlated function $\Gamma_0(q_1, q_2)$ (11) in reciprocal space:

$$\Gamma_0(q_1, q_2) = B_0\exp[-(Q_1+Q_2^*)] \times \exp[-(q_1-q_2)^2/q_C^2], \quad (20)$$

where $B_0 = r_0/(2\pi\gamma_0 q_0)$, $Q_{1,2} = (q_{1,2}/q_0)^2(1 + i\alpha_0)$, $q_0 = k_0\Delta\theta_0\gamma_0$ is the width of spectral density function $\Gamma_0(q, q) = B_0\exp[-2(q/q_0)^2]$. The width of angular spectrum $\Delta\theta_0$ depends on the size of incident beam r_0, the parameter of regular phase α_0, and the relation of beam size r_0 to LSC ρ_0 (see also [3]):

$$\Delta\theta_0 = (\lambda/\pi r_0)[1 + \alpha_0^2 + 2(r_0/\rho_0)^2]^{1/2}. \quad (21)$$

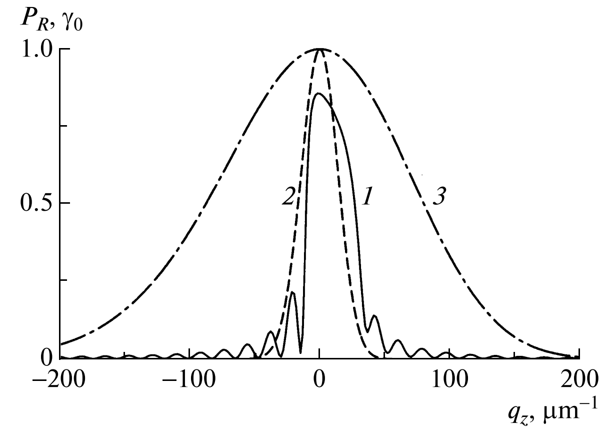

Fig. 1. Curve of diffractive reflection (*1*) and spectral densities $\gamma_0(q_z)$ for plane random waves with LSCs $\rho_0 = 0.1$ μm (*2*) and $\rho_0 = 0.02$ μm (*3*). Radiation CuK_α, $\theta_B = 1.14°$.

The value $q_C = q_0(\rho_0/r_0)$ in (20) defines the correlation rate of various spectral components of the field. It is easy to show that in the range of a very wide beam (at $r_0 \to \infty$), the width is $q_0 \to \sqrt{2}\Delta q_0$ where, as in (16), $\Delta q_0 = 2\gamma_0/\rho_0$ and value $q_C \to 2\sqrt{2}\gamma_0/r_0 \to 0$. Finally, taking into account the well-known representation for δ-function $\delta(x) = (1/\pi^{1/2}\xi)\exp[-(x/\xi)^2]$ at $\xi \to 0$, we find that ratio (20) for the beam transforms into $\Gamma_0(q_1, q_2) = \Gamma_0(q_1)\delta(q_1 - q_2)$ for the random plane wave, where $\Gamma_0(q_1)$ coincides with (16).

To get a simple analytical expression for SCF (10), we write the amplitude coefficient of Bragg reflection from the MS as $R(q) = R_0\exp[-(q/q_B)^2]$, where $q_B = k_0\Delta\theta_B\gamma_0$ and $\Delta\theta_B$ is the angular width of the curve of diffractive reflection (CDR). We then find from (10) and (17) that the regular amplitude of the reflected wave is also Gaussian:

$$A_R(x, z) = A_R\exp[-(\xi\gamma_0/r_1)^2(1 - i\alpha_1)], \quad (22)$$

where $r_1(z) = r_0(\mu_B\beta_1/\beta_0)^{1/2}$ is the transverse dimension of the reflected beam and the parameter $\mu_B = 1 + (\Delta\theta_0/\Delta\theta_B)^2$ is defined by the ratio of the width of angular spectrum of incident radiation (21) to the width of CDR. Here, $\beta_0 = 1 + \alpha_0^2 + 2(r_0/\rho_0)^2$; $\beta_1(z) = 1 + \alpha_1^2 + 2(r_0/\rho_0)^2/\mu_B$; $\alpha_1(z) = (\alpha_0 + \beta_0 D)/\mu_B$ is the parameter of the regular phase of the reflected field; $D = \lambda|z|/(\pi r_0^2\gamma_0)$ is a wave parameter describing the diffractive spreading of the reflected beam as distance $|z|/\gamma_0$ increases, and amplitude $A_R = R_0(\beta_0/\beta_1\mu_B^2)^{1/4}$. Correlation coefficient (7) of the reflected beam is also Gaussian, $\gamma_R(\rho) = \exp[-(\rho/\rho_1)^2]$, where LSC $\rho_1(z) = \rho_0\mu_B(\beta_1/\beta_0)^{1/2}$.

Let us discuss the change of LSC in reflected beam ρ_1, as compared to ρ_0 in dependence on ratio $\Delta\theta_0/\Delta\theta_B$. If $\Delta\theta_0 \ll \Delta\theta_B$, $\rho_1/\rho_0 = r_1/r_0 = S^{1/2}$, where $S = (1 +$

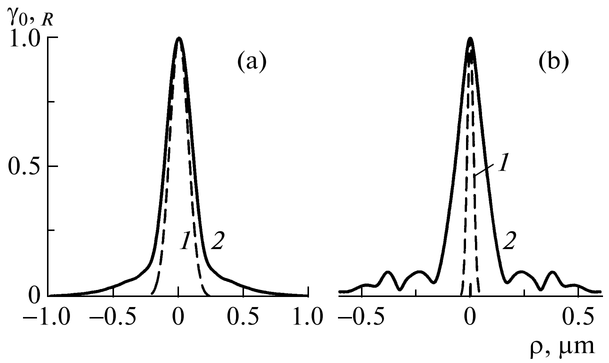

Fig. 2. Normalized functions of spacial coherence $\gamma_0(\rho)$ for incident (*1*) and $\gamma_R(\rho)$ for reflected (*2*) radiations; LSC of incident wave $\rho_0 = 0.1$ μm (a) and 0.02 μm (b).

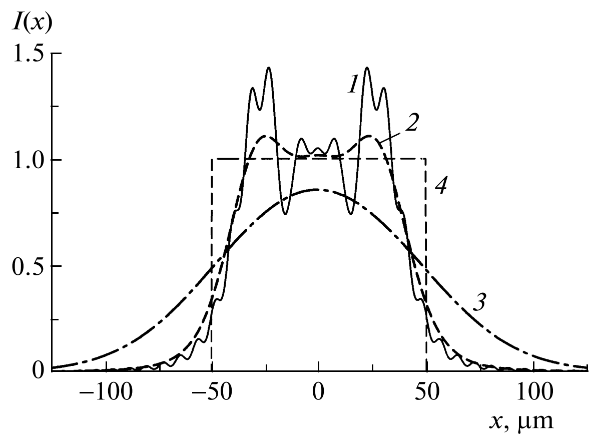

Fig. 3. Images of slit with dimension $r_0 = 50$ μm at LSCs $\rho_0 \to \infty$ (*1*), $\rho_0 = 20$ μm (*2*), and $\rho_0 = 5$ μm (*3*), and slit transmission function $S(x)$ (*4*). Distance $z = 5$ m; CuK_α is radiation.

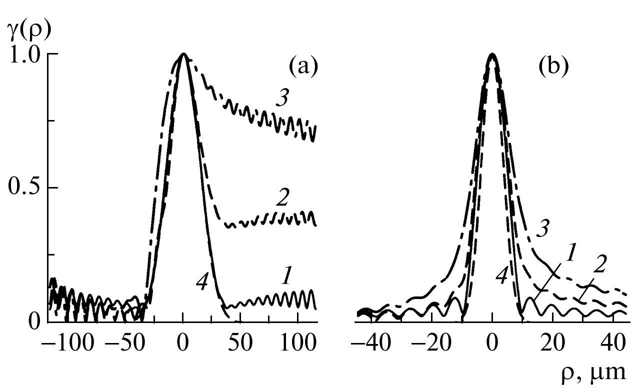

Fig. 4. Coherence degree $\gamma(x, x + \rho; z)$ in plane $z = 5$ m at points $x = 0$ (*1*), $x = 0.5r_0$ (*2*), and $x = 1.0r_0$ (*3*). Curves *4* are initial SCF $\gamma_0(\rho)$ with spatial coherence lengths $\rho_0 =$ 20 μm (a) and $\rho_0 = 5$ μm (b); slit half-width is $r_0 = 50$ μm.

$\alpha_0 D)^2 + D^2 + 2DW$, $W = \lambda|z|/(\pi\rho_0^2\gamma_0)$ (see also [3]). Beam spreading can be ignored if $|z|/\gamma_0 \ll L_F$, where $L_F = (\pi r_0^2/\lambda)[1 + 2(r_0/\rho_0)^2]^{-1/2}$. If, e.g., $r_0 = 30$ μm, $\rho_0 = 1$ μm, and $\lambda \approx 0.1$ nm, $L_F \approx 70$ cm. In the other extreme case of a strongly divergent beam (at $\Delta\theta_0 \gg \Delta\theta_B$), the value $\mu_B \gg 1$ and ratio $\rho_1/\rho_0 \approx \mu_B/\beta_0^{1/2}$. If a practically noncoherent beam with $\rho_0 \ll r_0$ falls on the MS, $\rho_1 \approx \rho_0(\Delta\theta_0/\Delta\theta_B)$; i.e., the LSC of the field of the reflected beam increases significantly in comparison with ρ_0. In the case $\alpha_0 \ll r_0/\rho_0$ the value $r_1(0) \approx r_0$ and $L_F \approx (r_0\rho_0/\lambda)(\Delta\theta_0/\Delta\theta_B)$.

We now examine the change in SCF shape (15) and LSC when a random plane wave with SCF $\Gamma_0(\rho') = \exp[-(\rho'/\rho_0)^2]$ is reflected from the MS. Figure 1 shows ideal plane wave CDR $P_R = |R(k_{0z} + q_z)|^2$ in the area of the first Bragg maximum $\theta = \theta_B$ and normalized spectral densities $\gamma_0(q_z) = \Gamma_0(q_z)/\Gamma_0(0)$ at two different values for the LSC of incident radiation ρ_0. More conventional argument q_z is connected with x-projection q in (15) and (16) by ratio $q_z = -q\cot\theta_B$. CDR was calculated by means of Parratt formulas [17], taking as an example MS W(0.1 nm)/C(0.3 nm) consisting of 40 periods and lying on a silicon substrate. Figure 1 demonstrates that in the case of weakly coherent radiation, only part of the wide angular spectrum (curve *3*) can effectively reflect from the MS in angular interval $\leq 2\Delta\theta_B$.

The results from calculating SCF of reflected radiation (15) are shown in Fig. 2. In the case of incident radiation with rather large LSC ρ_0, the shape of the SCF and LSC of reflected radiation are practically identical, except for the appearance of wide tails (Fig. 2a). Upon the Bragg reflection of radiation with relatively small LSC ρ_0, the integral length of the reflected wave's spatial coherency increases by a factor of 5 (Fig. 2b). It is more important here, however, that the shape of correlation function changes considerably; i.e., rather extensive oscillating wings appear (curve *2* in Fig. 2b). This clearly should be taken into consideration when using radiation reflected from an MS as the incident radiation on research subjects or other elements of X-ray optics (e.g., slits, multilayered mirrors, and crystals).

INFLUENCE OF THE SLIT ON THE SCF OF TRANSMITTED RADIATION

The model of partially coherent radiation with a degree of coherence in the form of Gaussian function $\gamma_0(\rho) = \exp[-(\rho/\rho_0)^2]$ is the one most common and is widely used in statistical optics [1] and the theory of X-ray image formation [2, 3, 9, 10, 15]. It is shown in this section that the slit limiting the beam (a mandatory part of all X-ray experiments) leads to local statistical inhomogeneity of the transmitted radiation, i.e., to the dependence of coherence degree $\gamma(x, x+\rho; z)$ on the coordinate of point x in plane z. These and other such matters are of interest when using synchrotron radiation sources, in which the distances between optical elements are measured in meters and tens of meters.

Let a plane random wave with amplitude $A_0(x)$, intensity $\langle|A_0(x)|^2\rangle = 1$ and SCF $\gamma_0(\rho)$ fall on a slit with function of transmission $S(x) = 1$ at $|x| \leq r_0$ and $S(x) = 0$ at $|x| > r_0$, where $2r_0$ is the overall slit width. The amplitude of the field in plane z is defined by Fresnel–Kirchhoff integral [16]

$$A(x,z) = \int_{-\infty}^{\infty} G(x-\xi)A_0(\xi)S(\xi)d\xi, \qquad (23)$$

where $G(x - \xi) = (i\lambda z)^{-1/2}\exp[i\pi(x - \xi)^2/\lambda z]$ is the Green function (free space propagator). Substituting (23) into (6) leads to the following expression for the SCF of radiation transmitted through the slit:

$$\Gamma(x, x+\rho; z)$$
$$= \int_{-r_0}^{r_0}\int_{-r_0}^{r_0} G(x-\xi)G^*(x+\rho-\xi')\gamma_0(\xi-\xi')d\xi d\xi'. \qquad (24)$$

Coherence degree $\gamma(x, x+\rho; z)$ is defined by ratio (7). If $\rho_0 \gg r_0$, transmitted field (23) may be considered completely coherent.

Figure 3 presents images of slit $I(x) = \Gamma(x, x; z)$ at various lengths of spatial coherence ρ_0. We can see that a reduction of ρ_0 leads to a smoothing and broadening of the image. Figure 4 shows that coherence degree $\gamma(x, x+\rho; z)$ of the radiation transmitted through the slit changes considerably in comparison with initial Gaussian function $\gamma_0(\rho)$. Side oscillations (curves *1*) appear in the central part of transmitted beam ($x \approx 0$). As we approach the edges of the slit ($|x| \sim r_0$, curves *2*, *3*), functions $\gamma(x, x+\rho; z)$ broaden, their shapes approaching the Lorentz function in the case $\rho_0 \ll r_0$ (Fig. 4b), and become sharply assymetric in the case $\rho_0 \leq r_0$ (Fig. 4a). Integral LSCs considerably exceed initial length ρ_0. A similar effect was predicted in [3] in the case of the Bragg reflection of a Gaussian beam from a crystal (see also paper [14] on experimental determination of the Lorentz form for the degree of coherence of undulator radiation transmitted through slits with various widths).

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