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X-ray scattering in capillary waveguides

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Abstract

In the past unexpected coherent phenomena associated with propagation of soft x-ray synchrotron radiation through capillary optical elements (polycapillary lenses and systems of capillaries) have been observed and investigated. In this letter theoretical analysis on x-ray scattering at grazing angles inside capillaries is presented.

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The possibility to deflect x-ray beams using the total external reflection from a surface was demonstrated for the first time by Compton [1] and Jentzsch [2]. However, technical difficulties to produce long and high quality optics working at grazing angles did not allow the growth of applications for decades. In particular, the influence of a surface roughness on parameters of the reflected beam is crucial for any x-ray optics. For typical glancing angles $\theta \simeq \theta_c/2$ (θ_c is the Fresnel's angle) the roughness value should not exceed, as a rule, $10 \div 50$ Å, a complex task to achieve on large reflecting surfaces.

In the last two decades significant improvements in the technology of surface processing allowed the manufacturing of new devices like x-ray reflective mirrors, multilayer interference mirrors, capillary optics, etc. [3]. Among these, capillary optics appears to be very promising in term of roughness. Indeed, the internal walls of the channels are formed at the expense of superficial forces of a wall tension, that results in very smooth internal walls. Nowadays capillary optics represents a well-established x-ray and neutron optical technique that allows experiments on large samples, or with small-size beams (millimeter order) to be performed on a much smaller scale than other x-ray optical devices [4–6]. These optical elements consist of hollow tapered tubes that handle neutral particles by multiple reflections from the inner surface of channels [7].

X-ray capillary optics relies also on the ability of a tapered and/or bent capillary channel to act as an x-ray waveguide [8]. In fact, there is the possibility for a beam in modal propagation to be deflected through a large angle by multiple reflections. This optic may be considered as a whispering-gallery x-ray device [9,10] (the whispering-gallery phenomenon has been discussed in details elsewhere [11–14]).

In this report we consider coherent and incoherent effects of x-ray scattering inside capillary channels for both smooth and rough wall surfaces.

It is well-known that reflection of an electromagnetic wave occurs on an extended area, which minimal size at sliding angles is defined by the ratio $(\Delta d)_{\|\min} \sim 4\pi c\omega/\omega_p^2$ (ω, the energy of field quantum; ω_p, the plasmon energy) that is much greater than the atomic distances. It means that the interaction occurs in a macro field characterized by a macroscopic dielectric permittivity $\varepsilon \simeq 1 - \omega_p^2/\omega^2$, which determines both the reflection and absorption characteristics. The coefficient of reflection is defined by the absorption of radiation in the upper layer, where the electric field penetrates, and estimated as $(\Delta d)_\perp \sim 2\pi c/\omega_p$ (typically, $(\Delta d)_\perp \approx 50$ Å). A general analysis shows, that for sliding angles less than the Fresnel's angle, the total reflection from surface is observed. In the framework of geometrical optics the scattering occurs in a specular (mirror) direction and exhibits a coherent character, while incoherent phenomena are associated to the absorbtion of radiation in the reflecting layer.

In a real case the undressed border is characterized by a roughness. It should be underlined, that the scattered radiation is distributed into the walls of a capillary as well as aside the hollow channel (basically, the dispersion occurs in solid angle 4π), affecting the radiation distribution behind a capillary. As a consequence, to determine the divergence of the radiation beam transmitted by a capillary we have to solve the wave equation taking into account the surface roughness [3,15,16]

$$\left[\nabla^2 + k^2 \varepsilon_0 \left(\mathbf{r}\right)\right] E\left(\mathbf{r}\right) = -k^2 \Delta\varepsilon \left(\mathbf{r}\right) E\left(\mathbf{r}\right) \ , \tag{1}$$

where $\Delta\varepsilon$ is the perturbation in the dielectric permittivity ε_0 of wall material induced by roughness, and $E\left(\mathbf{r}\right)$ is the function of radiation field.

An evaluation of Eq.(1) with the boundary conditions of a typical capillary channel shows that x radiation may be trapped in binding state mode by the capillary channel potential [10]. The channel potential acts as effective specular reflecting barrier, and then the effective transmission of radiation by hollow capillary tubes is revealed. However, the radiation propagation inside capillaries appears to be complex. While the main portion of radiation undergoes an incoherent diffuse scattering, the rest (usually small) comes from coherent scattering processes, extremely interesting to observe and to understand.

The scattering of electromagnetic radiation by a rough surface may be described within general (diffuse) scattering theory [17,18]. Using this theory, the relative scattered intensity into solid angle $d\Omega$, in the case of x-ray travelling in a capillary, is described, in the first-order approximation, by the matrix element:

$$P_{ab} \simeq \frac{\pi\omega^4}{c^4\theta_b} \left|D_{ab}\left(\theta_b, \varphi_b\right)\right|^2 \left|G_F\left(\theta_b, \varphi_b\right)\right|^2 \quad , \tag{2}$$

where $D_{ab}\left(\theta_b, \varphi_b\right)$ is the dipole function of $a \to b$ transition, and $G_F\left(\theta_b, \varphi_b\right)$ is the Fourier transformation of the roughness correlation function. Obviously, Eq.(2) allows also the divergences of x-ray beams propagating through capillary systems to be calculated.

As recently it has been shown, under scattering of x rays in capillary systems not all peculiarities can be described by geometrical optics[19]. On the contrary, application of the methods of wave optics reveals some details of the scattering process [20,21]. In the case of an ideal reflecting surface (neglecting roughness) the reflected beam is basically determined by the coherent scattering of radiation (for details see [10]).

Assuming the waveguide is a hollow cylindric tube, the field, where a wave propagates, may be written as $\varepsilon = 1 + \chi\left(r\right)\left(\varepsilon_0 - 1\right)$, where $\varepsilon_0 = 1 - \delta + i\beta$ (δ and β are real values describing the polarizability and the attenuation of radiation, respectively), and $\chi\left(r\right)$ is the unit step function. Solving the wave equation we are mainly interested to the edge region, which, in fact, defines the wave guiding character inside a channel ($r \simeq r_1$): $r = r_1 + \delta r, \quad \delta r \ll r_1$. Using asymptotic methods and expansion in a set of unknown parameter [22,23], it is possible to present the radiation field as $E(r,\varphi) = A(r_1,\varphi)\,u(\delta r)$, where the function $A(r_1,\varphi) \equiv f(\epsilon) \approx f_0(\epsilon_0) + f_1(\epsilon_1) + \ldots$ determines the reflection coefficient from the waveguide wall, i.e. $R(\varphi) = |A(r_1,\varphi)|^2$. In the coordinate system of the guide, the wave equation at the edge region is simplified to

$$(\Delta + \varepsilon_{eff})\; u(\delta r) = 0 \tag{3}$$

Here we introduced an "effective potential" ε_{eff} depending on the parameters ε, k and A-function. From this equation one obtains the expression for the relative radial part of wave function

$$u_m(\rho) \propto \begin{cases} \Phi_m(\rho) & , \quad \rho > 0 \\ \alpha \Phi'_m(0)\, exp(\alpha\rho) & , \quad \rho < 0 \quad (\alpha > 0) \end{cases} , \tag{4}$$

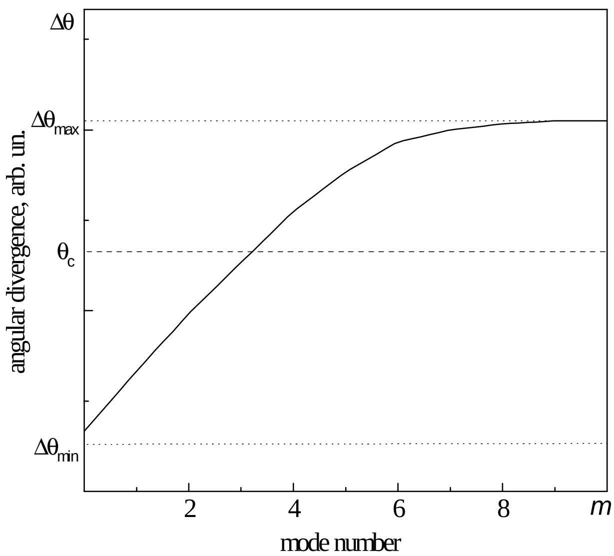

Figure 1: *Typical dependence of the angular divergence of a beam transmitted by a capillary channel vs the number of modes. Transition from a single-mode to a multi-mode propagation results in the increase of the angular divergence from* $(\Delta\theta)_{\min} < \theta_c$ *to* $(\Delta\theta)_{\max} > \theta_c$*, where* $(\Delta\theta)_{\max}$ *is limited by the capillary system design.*

where $\Phi_m(x)$ is the Airy function, and α is the arbitrary unit determined by the capillary wall material. This function characterizes the waves that propagates close to the waveguide wall, or, in other words, the equation describes the grazing modal structure of electromagnetic field in a capillary. The solution shows damping of the wave functions both inside the channel wall and moving away the wall towards the center. But almost total wave energy is concentrated in the vacuum region and, as a consequence, a small attenuation along the waveguide walls is observed. Note that, a modal propagation takes place without the wave front distortion due to coherent character of x-ray scattering by the effective potential. Additionally, the typical radial size $< u_0 > \simeq [(\lambda^2 r_1) / (2\pi^2)]^{1/3}$ of main grazing mode ($m = 0$) may significantly overcome the wavelength λ, whereas the curvature radius of "trajectory" r_1, may exceed the inner channel radius r_0: $< u_0 >\gg \lambda$.

Calculations of the angular distributions for different channeling modes indicates that in micron-size capillaries the divergencies of lower-number modes are less than the Fresnel's angle at any energy (Fig. 1). However, taking into account a large number of modes ($m \gg 1$) the divergence approaches upper limit mainly determined by a capillary system geometry. Studies on the divergence characteristics of x radiation passed through a capillary system represents independent interest and will be considered in the separate publication.

Consider the scattering by a rough surface. For simplicity, we introduce one-dimensional distribution of roughness $z = z(x)$ instead of two-dimensional real distribution $z = z(x, y)$, and also set $z = 0$ for a smooth surface. Then, the phase difference $\Delta\varphi = \mathbf{v}\ \mathbf{\Delta l}$ ($\mathbf{v}$, the propagating velocity; $\mathbf{\Delta l}$, the path vector) between two random rays scattered in the direction θ_s may be written as [17]

$$\Delta\varphi \simeq kL\left(\theta_s^2 - \theta_i^2\right) + \Re\left(z\right) \quad , \tag{5}$$

where L defines the reflecting surface dimension, $\Re\left(z\right)$ is the random function of surface roughness distribution $z = z(x)$, θ_i and $k = 2\pi/\lambda$ are the incident wave grazing angle and the wave vector, respectively. Since, typically $z_{\max} \ll 2L$, then $\Re\left(z\right) \ll kL\left(\theta_s^2 - \theta_i^2\right)$. Thus, we conclude that $\Delta\varphi \gg 2\pi$ for $kL\left(\theta_s^2 - \theta_i^2\right) \gg 1$, or, in other words, the field scattered by rough surface in the non-specular directions is always incoherent. Instead, for mirror-like reflection $\theta_s = \theta_i$, the phase of the wave may be present by the following

$$\varphi \simeq 2k\left(1 - \frac{\theta_i^2}{2}\right) z(x), \quad \theta_i \to 0 \quad , \tag{6}$$

that indicates: φ is constant for ideal smooth surface, hence, the field is coherent. From Eq.(6) one obtains the useful expression for coherence-incoherence analysis by means of variation technique (δ):

$$\delta\left\{\varphi\right\} = k^2\left(1 - \theta_i^2\right)\delta\left\{z\right\} \tag{7}$$

Let us now evaluate the ratio between the coherent and incoherent fields reflected by the smooth and very rough surfaces. As is well-known, the mean scattered power $P_s \propto \langle E_s E_s^* \rangle$ may be analyzed by the splitting: $\langle E_s E_s^* \rangle = \delta\left\{E_s\right\} + \langle E_s \rangle \langle E_s \rangle^*$, which determines the ratio between the scattered field and the mirror-reflected field. The two components of this relation characterize two different cases. When the surface is smooth, $\delta\{E_s\} = 0$, hence $\langle E_s E_s^* \rangle = \langle E_s \rangle \langle E_s \rangle^*$, i.e., only coherent waves will be reflected. On the contrary, when the surface is very rough, $\langle E_s \rangle \langle E_s \rangle^* = 0$, hence $\langle E_s E_s^* \rangle = \delta\{E_s\}$, i.e., only the incoherent waves are scattered. Between these two pure states of the reflected field, a continuous transition from coherence to incoherence is expected [24]. To determine the variance $\delta\{E_s\}$, the 2D surface distribution $\rho(z_1, z_2, \Delta z)$ (in other words, the $2D$ distribution of z at two points z_1 and z_2 separated by the distance Δz), has to be known. Obviously, the surface roughness may be regular or irregular in space.

Consider a periodical roughness $z(x) = z(x+a)$, where a is the period of the surface roughness profile along longitudinal capillary channel axis. From simple evaluation of general scattering relations we may obtain the dependence for incident and scattered angles: $(\theta_s)_m = \theta_i + m\lambda/a$. As a result, the diagram of dispersion, described by the expression

$$P = \sum P_m = \sum \frac{1}{I_{0m}} \frac{dI_m}{d\Omega} \propto \left| R_i(\theta_i) \sqrt{\varepsilon(\theta_i)} \right| \sum_m |\alpha_m|^2 \left| R_m(\theta_m) \sqrt{\varepsilon(\theta_m)} \right| \quad , \quad (8)$$

consists of narrow-forwarded peaks focused in the directions defined. Because of $m\lambda/a \ll 1$ in the x-ray spectral range, the dispersion will be maximal at small sliding angles $\theta_i \to 0$, so that

$$P \propto \theta_i \sqrt{\varepsilon(\theta_i)} \sum_m |\alpha_m|^2 \theta_m \sqrt{\varepsilon(\theta_m)} \quad , \quad (9)$$

where $|\varepsilon(\theta_i)| \simeq \theta_i^2 \pm 2m\lambda/a - (m\lambda/a)^2$.

Apparently, this dependence can be rather complex and exibits characteristic extrema. The main maximum appears in the mirror direction (coherent scattering), while the broadening of the observed angular distribution is due to the incoherent scattering. Note that for all considered angular ranges and roughness parameters the radiation dispersion is mainly observed at angles larger than the incident (Fig. 2). Actually, the coherent part of radiation, defined in Eq.(9) by the term before the sum, is distributed for all angles of dispersion, e.g. $\langle E_s(\theta) \rangle \langle E_s(\theta) \rangle^* \neq 0$. Moreover, the angular distribution of scattered radiation at small profile periods shows the tendency to increase dispersion towards large angles. In the dispersion there is also an additional maximum for angles larger than the incident angle due to the coherent component provided by the waviness of interaction potential: $\partial_\theta' \left(\langle E_s(\theta) \rangle \langle E_s(\theta) \rangle^* \right) |_{\theta=\theta_1>\theta_c} = 0$. However, the latter does not strongly affect the transmitted power by a capillary.

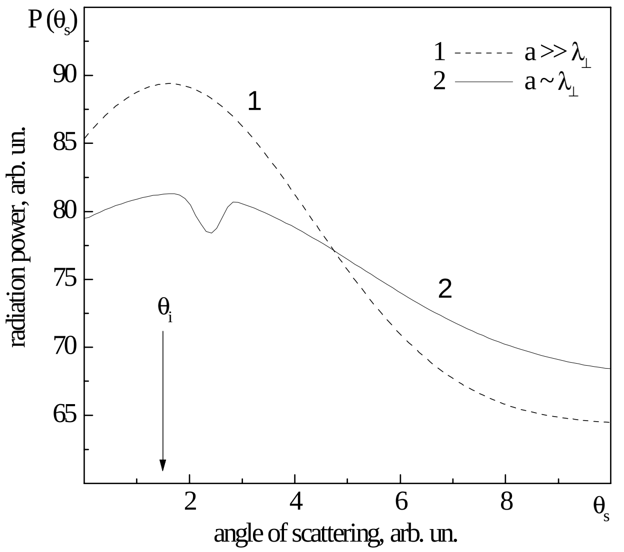

Figure 2: *Characteristic dependences of the angular distribution of scattered x radiation in capillary channels in the case of a periodic roughness perpendicular to the longitudinal channel axis: (1) roughness value much more than transverse wavelength of radiation:* $a \gg \lambda_\perp$*; (2) roughness value comparable to transverse wavelength:* $a \sim \lambda_\perp$ *(in our calculations only the distributions in the meridional plane are considered).*

The dispersion of x radiation at grazing incidence scheme due to an irregular surface roughness has been previously investigated [16]. Within the limits of grazing angles the dispersion was presented in the form

$$P_s(\theta_s) \propto (k\theta_i)^3 \left(\frac{\theta_s}{\theta_i}\right)^2 \frac{\left|\theta_i + \sqrt{\varepsilon - 1}\right|^2}{\left|\theta_s + \sqrt{\varepsilon - 1}\right|^2} R(\theta_i)\,\zeta(\theta_{si}) \quad , \tag{10}$$

where $k\theta_i \simeq (k_\perp)_i$ is the incident transverse wave vector, R is the Fresnel's coefficient, and ζ is the function defined by the surface roughness, $\theta_{si} \equiv (k_\perp)_i |\theta_s - \theta_i|$. The correlation analysis of Eq.(10) has been done assuming maximal dispersion in the mirror direction, i.e., $\theta_{si} = 0$. The results demonstrate that in the case of a single reflection from a rough surface the observed maximum coincides with the specular direction, or is displaced aside at an angle between the Fresnel's and specular angles. However, at small grazing angles ($\theta_i \to 0$) that typically takes place in capillary optics, a surface channeling phenomenon has to be introduced. The last substantially modifies the character of radiation distribution in channels. Morever, as mentioned above, due to the modal radiation propagation, the angular distribution shows a maximum at angles $(\theta_s)_{\max} \lesssim \theta_i$.

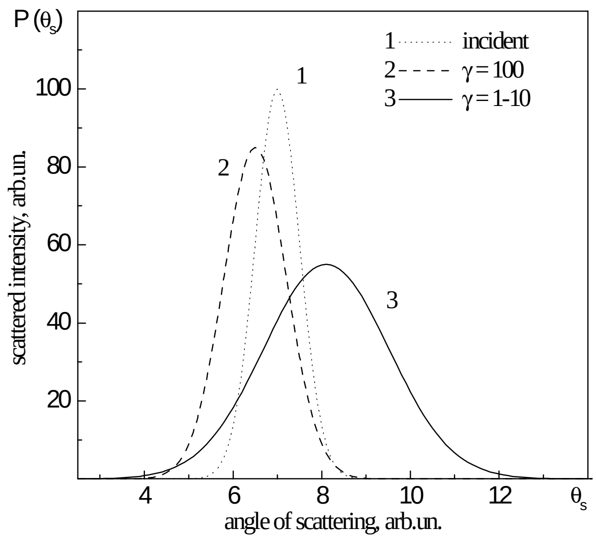

Figure 3: *Angular distributions of x rays inside capillary channel with rms height* $\xi = 25$ *Å. The dotted curve is the incident radiation distribution, while the dashed curve is the angular distribution of scattered radiation for roughness parameter* $\gamma = 100$. *The solid curve is given by* $\gamma = 1 \div 10$. *(The angles of scattering are less than the critical angle of total external reflection, and given in arbitrary units).*

Starting from the solution of Eq.(1) one may obtain the angular distribution of scattered radiation in capillaries. Calculations by general formulas for the scattered intensity [17] in the case of a correlation function $G(x) = \xi^2 \exp(-x/\sigma)$ for the smooth surface with rms height ξ and correlation length σ, result in the following dependence

$$P_s(\theta_s) \propto \frac{\xi^2 \sigma}{\theta_s \left(1 + (\sigma \Delta k)^2\right)^{3/2}} \sum_m |E_m(\theta_s)|^2 \quad , \tag{11}$$

where $E_m(\theta_s)$ is the angular function for the m-mode that produces the radiation distribution shown in Fig. 3. The angular distributions of scattered radiation are mainly affected by correlation lengths. The influence of roughness becomes essential, when the correlation lengths are of the order of transverse wavelength: $\sigma \sim \lambda_\perp \gg \lambda$ $(\gamma \equiv \sigma/\lambda_\perp \gtrsim 1)$, and, as a consequence, for definite roughness parameters a portion (not negligible) of radiation is scattered into angles less than the incident. It has to be underlined, that similar features may also take place in the case of a smooth wall surface. Such behavior is associated to a fraction of the radiation beam trapped in binding mode, i.e. in a surface channeling regime, while the remaining beam portion propagates through a channel in a diffuse scattering regime. Some features of radiation dispersion on surface roughness reported earlier [25] are confirmed by our analysis [26].

Evaluation of Eq.(11) shows also that, the scattering is mainly incoherent for $\gamma \lesssim 1$, i.e., $\langle E_s E_s^* \rangle \simeq \delta \{E_s\}$, although, the coherent component, that is negligible in view of capillary radiation transmittance, is still present ($\langle E_s \rangle \langle E_s \rangle^* \to 0$). When $\gamma \gg 1$, the coherent term increases and the scattering becomes partly coherent. In this limit, one may observe the small angular diffraction of reflected rays, as discussed by Compton [27], and in the distribution of scattered beam the features of coherent scattering may be recognized.

Recent x-ray and neutron research activities have shown that capillary/polycapillary optics is a powerful optical instrument useful for a number of applications [28]. However, a lot of work have still to be performed to clarify the mechanisms of radiation propagation inside these devices. We have discussed some effects still unclear, such as the influence of roughness on radiation propagation inside capillary systems. We conclude that the geometrical optics approximation is valid only, when the number of wave modes is large, and, as a consequence, the sum over separate modes may be replaced by the angular integration. It has been shown that, due to the surface channeling, the coherent dispersion can occur at angles less than the incident. We also indicate that the divergence of x-ray beam emerging by capillary system may be reduced, when specific correlation among parameters of x-ray beam and capillary channel is considered. Our results confirm that the guide of x rays over long distances is possible due to the lower-mode propagation mechanism through capillaries (see also [8]).

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