On the sensitivity of wave channeling of X-ray beam
to the shape of interface channels.

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Abstract

The using of microdiffraction of X-ray radiation for analysis of the structure of material specimens with submicron resolution becomes very promising investigation method [1]. One of the methods for obtaining of submicron beams of hard X-ray radiation is formation in a narrow channel of dielectrical resonator [1, 2]. In the present work the effect of transmission of X-ray through narrow submicron rough channels was investigated by numerical simulation with account for diffraction and decay of coherency. It was found that transmission can be strongly decreased for channels with periodic deformations. The effects of roughness were explained with the statistical theory of X-ray scattering in rough transitional layer. The wave mode attenuation coefficients $\beta$ scale as $\beta \sim 1/d^3$ ($d$ is channel width) and proportional to roughness amplitude $\sigma$. Possible explanation of observed anomalous energy dependence of transmission through thin Cr/C/Cr channel was given. The sensitivity of transmission of dielectrical channel to the presence of roughness and deformation with large space period was investigated.

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The using of microdiffraction of X-ray radiation for analysis of the structure of material specimens with submicron resolution becomes very promising investigation method [1]. One of the methods for obtaining of submicron beams of hard X-ray radiation is formation in a narrow channel of dielectrical resonator [1, 2]. Monitoring of X-ray beam by capture into a narrow dielectric channel is used in waveguide X-ray laser physics [3, 4], production of thin X-ray probe beams [2] and other applications [5] due to the effect of total external reflection.

In this work we consider the role of diffraction that can be important for narrow beams especially when roughness is high. Scattering from surfaces with high roughness needs special approach because small perturbation methods fail [6].

**Theoretical model**

X-ray scattering on rough surfaces is usually investigated within the well known Andronov-Leontovich approach [7] but for very small angles of incidence the model of "parabolic equation" for slowly varying scalar amplitudes of electrical field vector $A(x, z)$ should be used. Within the model scattering and absorption do not disappear at small grazing angle limit that results from Andronov-Leontovich approach [7]. In this case large angle scattering is neglected so

$$\partial^2 A(x, z)/\partial z^2 \ll k \cdot \partial A(x, z)/\partial z$$

and because the beam is narrow

$$\partial^2 A(x, z)/\partial z^2 \ll \partial^2 A(x, z)/\partial x^2,$$

where $z$ and $x$ are coordinates along and across the channel. The consideration will be restricted here to 2-dimensional channels (gaps) although the same approach can be applied to capillaries. The assumption results in "parabolic equation" of quasioptics [8]:

**
\[
2ik \frac{\partial A}{\partial z} = \Delta_{\perp} A + k^2 \frac{\varepsilon - \varepsilon_0}{\varepsilon_0} A
\]

\[A(x, z = 0) = A_0(x),\]  

(1)

where \( k = \sqrt{\varepsilon_0 \omega c} \). (In this case \( \varepsilon_0 \) is dielectrical permittance of air, \( \varepsilon_1 \) - dielectrical permittance of glass.) The evolution of the channeled X-ray beam was calculated by direct integration of the ”parabolic” equation \[9\]. The dielectric permittance on the rough boundary with the random shape \( x = \xi(z) \) was presented as

\[\varepsilon(x, z) = \varepsilon_1 + (\varepsilon_0 - \varepsilon_1)H(x - \xi(z)) \]

where \( H(x) \) is a step function. The distribution of roughness heights is assumed to be normal. It is known from results of \[7\] that at grazing incidence the effect of scattering is very small. So special surfaces are needed to observe scattering effects in the gap interface at reasonable distance. In the calculations we used roughness amplitude up to 400Å. The reflection of X-ray beam on very rough surfaces (up to 1500 Å) of silicon was observed in \[10\]. The results of direct simulation of scattering with the model rough surface by integration of equation (1) calculated for X-ray energy \( E = 10\text{keV} \), width of the channel \( d = 0.5\mu m \), \( \sigma = 400\text{Å} \) and correlation length of roughness \( z_{corr} = 5\mu m \) averaged over 40 realizations are shown on Fig.1 as normalized to initial value total intensity of the beam \( r_{tot} \), incoherent part \( r_{inc} \), where \( r_i = \int_{-\infty}^{\infty} I_i(x)dx/\int_{-d/2}^{d/2} I_0(x)dx \). Initial angles of incidence of plane wave were \( \vartheta = 0; 3 \cdot 10^{-4} \) and \( 6 \cdot 10^{-4} \text{rad} \) (Fresnel angle \( \vartheta_F = 3 \cdot 10^{-3} \text{rad} \)). The atomic scattering factors used in the calculations were taken from \[11\].
Evolution of the total integral normalized intensity of the beam $r_{tot}$ and normalized incoherent part $r_{part} = r_{inc}/r_{tot}$ for different incidence angles $\vartheta$. $\vartheta = 0, r_{tot}$ (curve 1), $r_{part}$ (curve 1'); $\vartheta F/10$ (curves 2 and 2'); $\vartheta F/5$ (curve 3 and 3').

The main result of direct simulation is that the loss of coherency comes along with attenuation of the beam and in the transmitted beam the coherent part prevails [8].

Analytical results for transmission of coherent part of X-ray can be obtained with statistical averaging of equation (1) using Tatartsky method (see [12]) as it was made in [8] by generalization of the method for stratified media. The same generalization of the method to include stratified media was used in the case of electron channeling in single crystals [13]. The method results in additional attenuation of coherent part of the amplitude $< A >$ due to ”scattering potential” $W(x)$.

$$W(x) = (-ik/4) \int_{-\infty}^{\infty} < \delta \varepsilon'(x,z) \delta \varepsilon'(x,z') > dz'$$

As it was shown in [8] ”scattering potential” can be expressed as
\[ W(x) \approx -\frac{k(\varepsilon_0 - \varepsilon_1)^2}{4\pi(\varepsilon_0)^2} \int_{-\infty}^{\infty} dz' \int_{-\infty}^{0} exp(-\xi^2) d\xi \int_{0}^{R(z')^2} exp(-\eta^2) d\eta \cdot exp(-\frac{x^2}{\sigma^2}) \] (2)

with clear dependence on vertical coordinate \( x \) where \( R(z) \) is the autocorrelation coefficient, \( \sigma \) is dispersion of \( \xi(z) \) distribution.

The decay of coherency for particular wave modes can be described with attenuation coefficients \( \beta_l \). Attenuation coefficients can be found as overlap integrals

\[ \beta_l = -\frac{k}{2} \int \varphi_l^*(x)[\text{Im}(\chi(x)) + W(x)]\varphi_l(x) dx, \]

where eigenfunctions \( \varphi_j(x) \) are solutions of equations

\[ \Delta_\perp \varphi_j(x) = k[2k_{jz} - k\text{Re}(\chi(x))]\varphi_j(x). \]

Statistically averaged refraction and absorption are accounted for by normalized term

\[ \chi(x, z) = (<\varepsilon(x)> - \varepsilon_0)/\varepsilon_0. \]

It can be shown for lower channeled modes that incoherent scattering attenuation coefficient is proportional to \( \sigma \) (see discussion above about dependence of \( W(x) \) on \( \sigma \))

\[ \beta_{\text{scatter}} \sim k^2(\varepsilon_0 - \varepsilon_1)^2 \sigma \int_{-\infty}^{\infty} d\xi' \int_{-\infty}^{0} exp(-\xi'^2/2) d\xi' \int_{0}^{R(z')^2} exp(-\xi'^2/2) d\eta. \]

The proportionality of losses of beam intensity to roughness amplitude \( \sigma \) under small gliding angles was obtained also in the numerical simulation results ([14], Fig. 5).

**Results**

The dependence of attenuation coefficients \( \beta \) of X-ray beam on the channel width \( d \) between silicon plates for three lower modes were shown in [13] and demonstrate \( \beta \sim 1/d^3 \).
dependence. Such dependence accounts for decreasing of diffractional effects with beam width $\sim \lambda/d^2$ and the effective portion of the beam that interacts with the surface $\sim \sigma/d$.

When lead plates were taken into consideration instead of silicon the value of attenuation coefficients became 1.5 times greater. Increasing of $\beta$ with decreasing of energy is stronger than $\sim 1/E$ that can be accounted for by increasing of diffraction along with increasing of optical density of channel walls.

Recently published experiments with Cr/C/Cr channel with length $L = 3\, \text{mm}$ and width $d = 1620\, \text{Å}$ of carbon layer had shown nonmonotonous energy dependence of transmission for '0' wave mode (Fig.2, rombs). As it was supposed roughness of the interfaces couldn’t exceed $\sim 10\, \text{Å}$.

![Fig.2.](image)

Calculated dependence of basic '0' wave mode transmission $T$ in Cr/C/Cr channel on X-ray energy. $L = 3\, \text{mm}$, $d = 1620\, \text{Å}$. Deformation amplitude $a = 120\, \text{Å}$, period $\Lambda = 100\, \mu\text{m}$ (curve 1), 500$\, \mu\text{m}$ (2), 1000$\, \mu\text{m}$ (3). $\sigma = 0\, \text{Å}$. Experimental points of W. Jark et al [2] are shown by rombs.

Direct numerical simulation of the transmission of X-ray beam with equation (1) was
developed to investigate the dependence of '0' and '1' modes transmission on roughness amplitude. The account for roughness decreases transmission of the basic mode with $E = 17keV$ by 1.3 % for $\sigma = 10\text{Å}$ and by 5 % for $\sigma = 20\text{Å}$ (see Fig.3) that cannot explain prominent depression of experimental results on Fig.2.

Fig.3

Dependence of transmission of 17 keV X-ray beam in the channel Cr/C/Cr width C layer $d = 1620\text{Å}$ for modes '0' and '1' on roughness $\sigma$, $z_{corr} = 5\mu m$.

For the expansion of anomalous dependence of 17keV radiation basic mode transmission through Cr/C/Cr channels periodic deformation of the layers were taken into account. The results are shown on Fig.2 for deformation amplitude $a = 120\text{Å}$ and periods $\Lambda = 100\mu m$ (curve 1), $500\mu m$ (2) and $1000\mu m$ (3).

The dependence of transmission on deformation period $\Lambda$ for $E = 17keV$ $a = 120\text{Å}$ and without roughness (the effect of roughness was not important; see Fig.3 above) is shown on Fig.4. Several resonances can be recognised in short $\Lambda$ region. So the results shown on Fig.2 and Fig.4 are similar to the complicated effects of strong wave function transformation of channeled electrons in superlattices [9].
Thus the depression of the transmission for $E = 17 \text{keV}$ on Fig.2 observed in [2] can be result of the periodic corrugation of Cr/C interface and wave mode interference.

To clear out the mechanism of decay of x-ray beam in thin film waveguide with periodic perturbations both decay of total intensity and basic mode "0” intensity on the distance was investigated for different periods $\Lambda$.

In the case of small scale perturbations ($\Lambda \leq 45\mu m$) basic mode intensity decreases nearly the same as the whole beam. And in the case of resonant perturbation $\Lambda = 45\mu m$ the intensity of basic mode is subjected to strong oscillations with the period $\Lambda/2$, decreasing at the distance $z = 3000\AA$ to 0.03 part of the initial value. In the nonresonance case $\Lambda = 40\mu m$ the basic mode "0” oscillations are substantial only near the entrance to the carbon channel. Intensity at the distance $z = 3000\AA$ on exit of the channel decreases to 0.6 of the initial value.

For the period ($\Lambda = 1000\mu m$) the dependence of total intensity and basic mode "0” intensity are shown on Fig.5 with curves 2 (points) and 2' (solid). Curves 1 and 1' correspond to the direct channel. Pulsations on the curve 1’ are due to calculation uncertainties. From the Fig.5 it is seen that in the case of large scale perturbations the decreasing of total intensity slightly differs from the straight channel. But decreasing of basic mode having the oscillation manner with the period $\Lambda/2$, may reach nearly 0.1 of the initial value. That is why the influence of large scale perturbations must result in substantial increasing of angular spread of the beam at the exit of the channel.

Discussion

The investigations developed show strong influence of deformations of the channel on the transmission of x-ray channeled beams. Small scale random perturbations of the surface with the roughness amplitude up to $20\AA$ do not effect considerably the transmission
of X-rays in comparison with diffraction effects that determine the decay of intensity in the channel in the case. The X-ray transmission is the most sensitive to the resonant periodical perturbations of the channel corresponding to the pendulum oscillations of modes ”0” and ”1”. In this case nearly complete dempening of the beam due to transfer of basic mode ”0” to upper modes which decay rapidly [8, 15]. In the case of large periods of deformations of the channel effective transfer of the beam to the higher modes takes place but it do not succeed in substantial change of total intensity. It is worth noting that the effect of abnormal energy dependence of transmission of the beam through Cr/C/Cr channel that was observed in [2] dissapeared after the technology of production of X-ray waveguides was improved [16] that can serve as the confirmation of the results of the present work.

The results of the present work can be used for creation of new type of tunable X-ray filters for formation of thin beams of synchrotron X-ray radiation.

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The dependence of basic '0' wave mode transmission $T$ of $E = 17keV$ X-ray beam in Cr/C/Cr $d = 1620\,\text{Å}$ channel on the deformation period $\Lambda$. $\sigma = 0\,\text{Å}$, $L = 3\,\text{mm}$, $a = 120\,\text{Å}$.
The evolution of total intensity (curves 1 and 2, point) and basic mode "0" (curves 1' and 2') of X-ray beam with energy $E = 17keV$ in the channel Cr/C/Cr, $d = 1620\,\text{Å}$ for direct channel (1 and 1') and under deformations with the period $\Lambda = 1000\,\text{µm}$ (2 and 2').

$\sigma = 0\,\text{Å}$, $L = 3\,\text{mm}$, $a = 120\,\text{Å}$. The initial beam corresponds to the basic waveguide mode.