MATHEMATICAL SIMULATION OF X-RAY OPTICAL SYSTEMS USING MONTE CARLO METHOD

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Résumé - On a effectué une simulation mathématique des systèmes
d'optique des rayons X à cristaux à double courbure. On a mon-
tré que les courbes de rendement de réflexion des cristaux à
double courbure pour le cas d'une source ponctuelle possèdent
deux maxima : $R_2/R_1 = 1$ (sphère) et $R_2/R_1 = \sin^2\theta_0$ (surface en
forme de tonneau à focalisation ponctuelle). Des cristaux
sphériques sont recommandés pour des montages de rayons X à
fentes (diaphragmes).

Abstract - There is performed mathematical simulation of
X-ray optical systems with double-bent crystals. It is shown
that curves of reflection efficiency for double-bent crystals
have two maxima at $R_2/R_1 = 1$ (sphere) and $R_2/R_1 = \sin^2\theta_0$
(barrel-shaped surface with point focusing) when using a point
radiation source. For X-ray optical systems with slit sources
(diaphragms) it is advisable to use spherical crystals.

To compute parameters of complex X-ray optical systems (efficiency,
resolution, aberrations, tolerances for manufacture and arrangement
of system components and so on) we applied a technique of mathemati-
cal simulation by Monte Carlo method /1,2/. The developed technique
was used for computation of X-ray optical systems with double-bent
crystals which are of high interest in development of X-ray spect-
rometers of high efficiency /3,4/. In the present work there was
studied distribution of reflecting areas and reflection efficiency
for crystals bent along surfaces created by rotation of an arc of
radius R_1 lying in a focal plane around an axis lying in the same
plane. In this case a central point of the arc has rotation radius
R_2. It was assumed that reflecting planes of the crystal are paral-
lel to its surface.

When trajectory of a photon is assigned as a straight line passing
via the point radiation source and current point on the crystal sur-
face, a glancing angle θ complementary to the angle between photon
trajectory and normal to the crystal surface in the current point
may be found. For those points on the surface under study which are
located at random or as a net there was computed angle θ and deter-
mined difference between this angle and Bragg angle θ_0. As a result
of computation there was obtained a net listing (topogram) with sym-
bols of three types of points corresponding to the following cases:

$$(\theta - \theta_0) > \delta/2 , \quad \delta/2 \geqslant (\theta - \theta_0) \geqslant -\delta/2, \quad (\theta - \theta_0) < -\delta/2$$

where δ is a crystal mosaic. The second case corresponds to ref-

lection. Then there was computed a value of solid angle Ω at which
a reflecting area is seen from the source (reflection efficiency).
In Fig. 1 there is shown succession of topograms for various values
of $\varphi = R_2/R_1$. Reflecting areas of the surface are black, areas with
value O corresponding to the first case are marked by sign " - " and
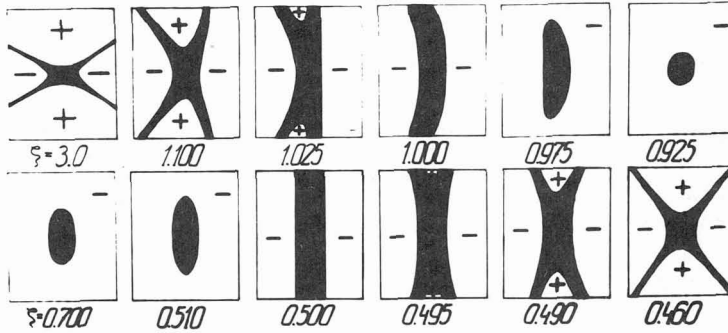those corresponding to the third case are marked by " + ".

Fig. 1 - Topograms of crystal surface (height h/R_1 =0.4, width
b/R_1 = 0.2) for different values of $\varphi = R_2/R_1$ with 0_0=45°, δ =
0.00058. Source is located in focal plane.

As it is seen from the figure for large values of φ the topograms
correspond to Iohann focusing. As the surface shape approximates to
a sphere a cross is transformed in a slightly bent vertical belt.
Then with decrease of φ this belt is compressed in an elliptical
spot which is again extended along the vertical changing at φ =
0.5 $\mathrm{Sin}^2 45°$ into a straight closed vertical belt corresponding to
the condition of point focusing at the barrel-shaped surface /4/.
With the further decrease of φ a cross similar to the initial one
appears again. It may be shown analytically that the height of ref-
lecting area in the center of crystal has two maxima (at φ = 1 and
$\varphi = \mathrm{Sin}^2 0_0$) corresponding to the crystal bending along the sphere
and barrel-shaped surface with point focusing (Fig. 2).

When the reflecting surface is obtained by rotation of logarithmic
spiral arc or the crystal is made according to Iohansson the above-
mentioned dependence is a characteristic of reflecting area height
of the whole crystal, i.e. of its efficiency. Reflection efficiency
as a function of φ for the case shown in Fig. 1 is represented in
Fig. 3. As it is seen from Fig. 3 there are 2 typical maxima of ref-
lection located near to φ =1 and φ =0.5. The latter maximum is nar-
row enough and so there are high requirements to the accuracy of R_2.
Requirements to the accuracy of R_2 when bending along the sphere
are considerably lower. Similar computations for other values of Θ_0
show that the general behaviour of reflection efficiency curves is
reserved (maxima are near to φ =1 and $\varphi = \mathrm{Sin}2\Theta_0$) , these maxima
are sharpened with the decrease of Θ_0.

In Fig. 4 there are shown crystal surface topograms in case of sour-
ce displacement along a normal to the focal plane for values $\varphi = 0.5$
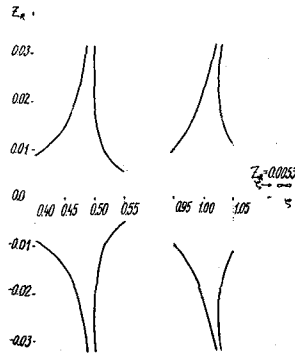and φ = 1. Corresponding curves of reflection efficiency are shown

Fig. 2 - Reflecting area height $Z_R \approx Z/R$ (in direction of normal to focal plane) as a function of ζ for conditions shown in Fig. 1.
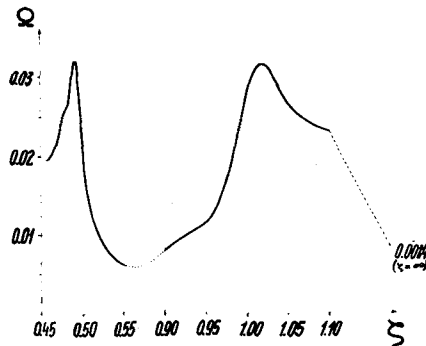

Fig. 3 - Reflection efficiency Ω as a function of ζ for conditions shown in Fig. 1.

in Fig. 5. As it is seen from Figs.4 and 5 arrangements with crystals bent along the barrel-shaped surface with point focusing are extremely critical to displacement of the point source along the normal to the focal plane that hampers the use of slit sources. Unlike this case for the systems with spherically bent crystals it is possible and advisable to use slit sources. Computations for other values of Θ_o confirm these conclusions.
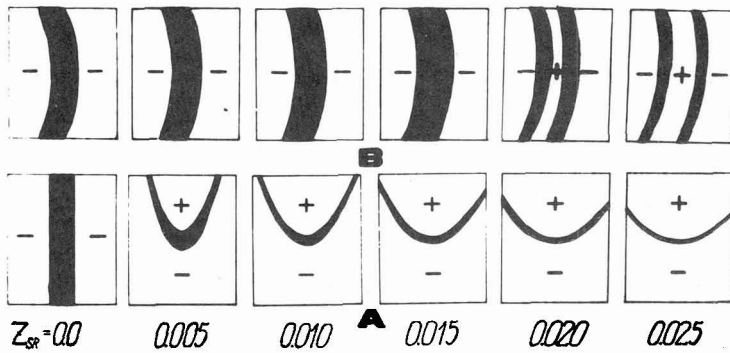
Fig. 4 - Surface topograms of the same crystal for various displacements of the source ($Z_{SR} = Z_S/R_1$) along normal to focal plane with $\varUpsilon = 0.5$ (A) and $\varUpsilon = 1$ (B).
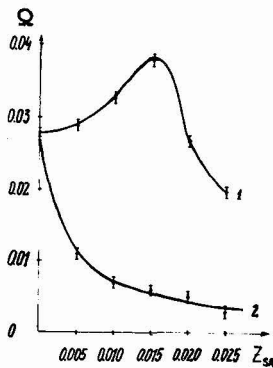

Fig. 5 - Reflection efficiency of the same crystal as a function of Z_{SR} with $\varUpsilon = 1$ (1) and $\varUpsilon = 0.5$ (2).

References

1. PLOTNIKOV R.I. et al., Apparatura i metody rentgenovskogo analiza 23 (1980) 27.

2. PLOTNIKOV R.I. et al., Apparatura i metody rentgenovskogo analiza 28 (1982) 42.

3. EGGS J.U., Z. angew. Phys. 20 No.2 (1965) 118.

4. BERREMAN D.W. et al., Rev. Sci. Instr. 25 (1951) 1219.