

Program vkCRLpar

The parameters of x-ray beam passing the system of CRLs

V. G. Kohn, Kurchatov institute

This program is a part of more general program **vkUtility.jar**. The latter can be downloaded from it's web page [4]. The program can be opened by clicking the button [Science] and then [CRLpar].

1. The task and input data

The program calculates the parameters of the Gaussian beam which goes from the source to the detector through a system of CRLs (compound refractive lenses). Calculations are based on the recurrent relations which was derived in the papers [1–3]. It is assumed that CRL consists of $N > 1$ chips (simple refractive biconcave lenses) which have an aperture A and a length p including a free space near the lens. The free space is small so that the chips are packed closely. The experimental setup may contain many CRLs with an arbitrary distances between them. Each CRL is characterized by the distance behind it. The distance of last CRL is the distance to the detector, see figure 1.

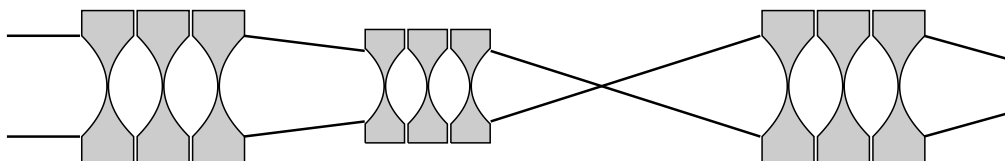


Fig. 1. A scheme of CRL system.

The program assumes the 1D (planar) CRL. However, the results can be used for 2D (circular) CRL too. The rules how to use the results for 2D CRL is presented in section 4. A set of input data includes first the following 5 parameters, each in a separate line:

Energy E of the radiation photons in keV

Source transverse size w_s in microns

Angular divergence α_0 of the beam from the source in microradians

Distance z_0 from the source to the beginning of the first CRL in the system in cm

Number N_0 of CRLs

The next 8 lines must contain N_0 values (array) for each CRL individually and these values may be different. The values have to be separated by one or more blank symbols. They are the main parameters of the CRL, namely,

Chemical formula like FeBO(3) i.e. one or two symbols for element and a number in brackets

Density of matter in gram per cubic cm

Linear Aperture A in microns

Curvature radius R at the apex of parabola in microns

Length p of one biconcave chip in microns including the empty space near it

Web thickness d in microns as a thin layer between two parabolas

Number of chips N in one CRL

Distance z_1 between this and next CRL in cm. For last CRL next one is a detector.

We note that the recurrent relations are used for each chip inside CRL. Only one chip of CRL is considered as a thin lens. That allows one to obtain correct results even for one long CRL which can focus the beam at their end or inside it. The program takes into account accurately the angular divergence of the incident beam. It is assumed that module of the wave function decreases with the angle according to the Gauss law.

This means that the wave function of the radiation in front of the first CRL has a form $P(x - x_0, b_0)$ where

$$P(x, z) = \frac{1}{(i\lambda z)^{1/2}} \exp\left(i\pi \frac{x^2}{\lambda z}\right), \quad b_0 = z_0 \left(1 + i\frac{\sigma}{z_0}\right)^{-1}, \quad \sigma = e_1^2 \frac{\lambda}{\alpha_0^2}. \quad (1)$$

Here $P(x, z)$ is a Fresnel propagator, $\lambda = 12.3984/E$ is a wave length in Angstroms, $e_1 = (2 \ln 2/\pi)^{1/2} = 0.6643$. The transmission function of one chip has a standard form

$$T(x, a) = \exp\left(-i\pi \frac{x^2}{\lambda a}\right), \quad a = \frac{f}{1 - i\gamma}, \quad f = \frac{R}{2\delta}, \quad \gamma = \frac{\beta}{\delta} \quad (2)$$

This function is applied for all chips except first one. The first chip takes into account the aperture A of the CRL. In this case the parameter a contains $\gamma + \lambda f/(2A^2)$ instead of γ .

2. The output data

In our approximation the transverse intensity distribution of the beam for each distance from the source is the Gauss function

$$I_{ps}(x, x_0) = \frac{z_t}{|b|} \exp\left(-\frac{x_0^2}{2\sigma_0}\right) \exp\left(-\frac{(x - x_m)^2}{2\sigma^2}\right), \quad (3)$$

where x_0 is a coordinate of a point on the source, $x_m = -Mx_0$ is a coordinate of the beam center. The parameter FWHM (full width at half maximum) is equals to $w = e_2\sigma$, $e_2 = (8 \ln 2)^{1/2} = 2.3548$. We consider three distances (1) just behind the last CRL, (2) at the focus distance behind the CRL, (3) at the detector distance. It can be shown that at the distance z_1 behind the last CRL $M = (z_1 + Z_1)/(z_0 + Z_0)$.

The output data are presented in the text file [results.txt] which is shown in the window of text editor. First of all the input data are presented in the compact form of array of numbers in the order as they appeared in the input windows. Then a global parameters are shown as (1) The focus distance counted from the end of last CRL, (2) The web absorption as the multiplier due to absorption on the thickness between two parabolas of each chip (3) The effective aperture and length of CRL. The last two parameters have a sense only in the case of one CRL. We note that the effective aperture is the same as the relative integral intensity but without taking into account the web absorption.

Then the data for the point source are presented. (1) The integral relative intensity, including the web absorption. Relative intensity is calculated relative the distance z_t from the source to the end of last CRL. (2) The rocking curve FWHM in microradians. It is calculated as a ratio w_0/z_0 where $w_0 = e_2\sigma_0$. (3) The parameters Z_0 and Z_1 which allows one to calculate a shift of intensity pick from the optical axis. Then two parameters: maximum relative intensity as $z_t/|b|$ and FWHM w are shown for three distances pointed above.

After this information the same data for the real source are presented. The brightness of the source is described by Gaussian

$$B(x_0, x_s) = \frac{1}{\sigma_s(2\pi)^{1/2}} \exp\left(-\frac{(x_0 - x_s)^2}{2\sigma_s^2}\right) \quad (4)$$

where $\sigma_s = w_s/e_2$, w_s is the source size as it is determined in the input data, x_s is a shift of the source center from the optical axis which is used for a description of the rocking curve. The intensity distribution is determined as

$$I_{rs}(x, x_s) = \int dx_0 B(x_0, x_s) I_{ps}(x, x_0) \quad (5)$$

The integral is calculated analytically with the result

$$I_{rs}(x, x_s) = I_m \exp\left(-\frac{x_s^2}{2\sigma_2^2}\right) \exp\left(-\frac{(x + M_s x_s)^2}{2\sigma_1^2}\right) \quad (6)$$

where

$$\sigma_2 = (\sigma_0^2 + \sigma_s^2)^{1/2}, \quad M_s = MC, \quad \sigma_1 = (\sigma^2 + M^2 C \sigma_s^2)^{1/2} \quad (7)$$

$$C = \frac{\sigma_0^2}{\sigma_2^2}, \quad I_m = \frac{z_t}{|b|} C^{1/2} \frac{\sigma}{\sigma_1} \quad (8)$$

The program shows the same parameters as for the point source. Very often the integral intensity has approximately the same value as for the point source. We can write for the integral intensity

$$S_{rs}(0) = S_{ps}(0)C^{1/2}, \quad S_{ps}(0) = (2\pi)^{1/2} \frac{\sigma z_t}{|b|} \quad (9)$$

It follows from the formulae that this fact takes place if $\sigma_0 \gg \sigma_s$. As for the rocking curve FWHM, now it is calculated as a ratio w_2/z_0 where $w_2 = e_2\sigma_2$.

3. Details of implementation

Figure 2 shows the input window of the program. It contains the five buttons. The button [OK] runs the calculation. The button [Cancel] stops the program working. The program remembers the input data for a current variant. However, the user has a possibility to save the current input data to one of 52 cells of storage memory and then restore the saved variant. These operations are possible by clicking the buttons [Save Var] and [Choose Var]. After clicking these buttons the user has to select the index of variant where the data will be remembered or restored. The button [Notes] allows user to write any information to the file [difpar.txt] of the program folder [s/vkDifPar], in particular, the information about saved variants. The button [Help] opens this file in the browser.

Figure 3 shows the output window of the program. The results of calculation are a set of parameters of the x-ray beam which is saved to the file [results.txt] in the program folder [s/vkCRLpar] and then the file contents is shown on the screen inside the window of the text editor. This file is changed in each run of the program. Therefore to save the specific results, the file has to be copied to the file with other name by means of some file manager, for example, [Total Commander], [Q-Dir], Windows file manager, or vkUtility operation.

4. How to obtain the results for 2D (circular) CRLs

The program is managed on the idea of the paper [3] where an approximate account of the aperture is proposed. In this approximation the 2D transverse intensity distribution is equal to a product of two 1D intensity distributions along the x and y coordinates, namely,

$$I_{rs}(x, y, x_s, y_s) = I_{mx}I_{my} \exp\left(-\frac{x_s^2}{2\sigma_{2x}^2} - \frac{y_s^2}{2\sigma_{2y}^2}\right) \exp\left(-\frac{(x + M_{sx}x_s)^2}{2\sigma_{1x}^2} - \frac{(y + M_{sy}y_s)^2}{2\sigma_{1y}^2}\right) \quad (10)$$

where the fact is taken into account that the source size can be different for x and y coordinates. Therefore for a calculation of system of 2D circular CRLs it is sufficient to calculate the 1D variant for x and y coordinates separately and then to consider a product.

One note has to be done about the effective aperture. For the 2D CRL the effective aperture is determined by a diameter of the circular aperture D which can be obtained from the linear aperture A according to the relation $A^2 = \pi D^2/4$. Therefore $D = (2/\pi^{1/2})A$.

References

- [1] Kohn V. G., J. Surface Investigation, 2009, vol. 3, N. 3, p. 358-364
- [2] Kohn V. G., J. Synchr. Rad. 2012, 19, N.1, 84-92.
- [3] Kohn V. G., J. Synchr. Rad. 2017, will be published.
- [4] <http://kohnvict.ucoz.ru/vkacl/vkUtility.htm>

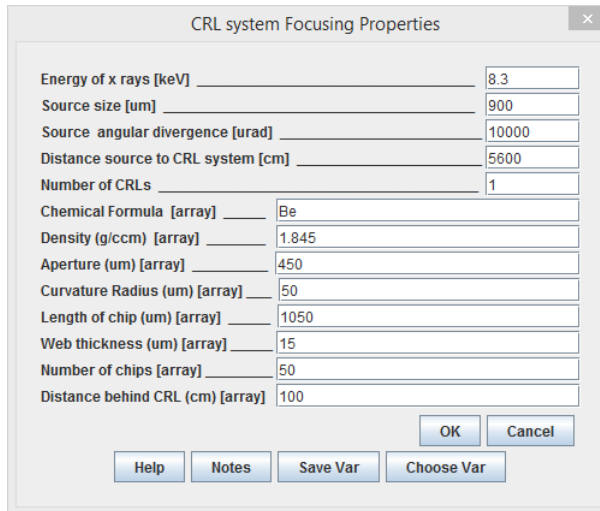


Fig. 2. The input window of the program

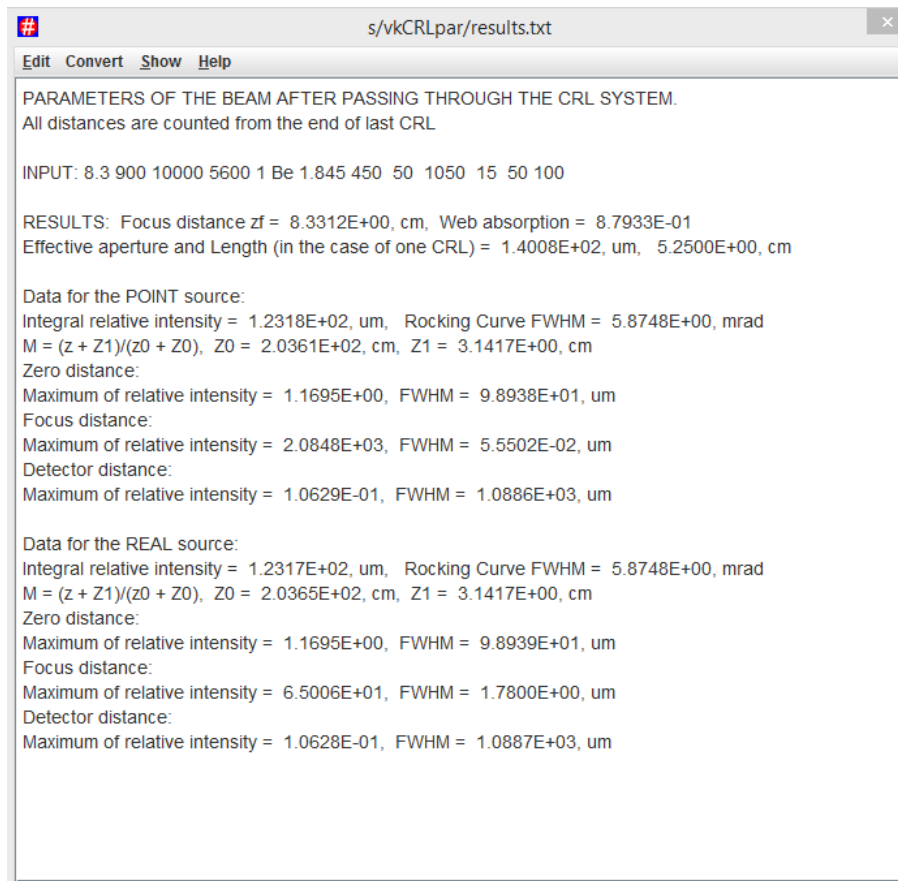


Fig. 3. The output window of the program