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NANOPHOTONICS

A New Version of the Theory of Nanofocusing Hard Synchrotron Radiation Beams by a Long Compound Refractive Lens. II

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Abstract—Two aspects of a new theory for nanofocusing synchrotron radiation (SR) into nanometer-scale transverse dimensions using a long compound refractive lens (CRL) are considered. First, a method for calculating the rocking curve, which differs from the Gaussian function and depends on the actual aperture size of the CRL, is developed. Second, a new method for calculating the wave function transformation as SR passes through air after focusing in the CRL, including in the region near the focal length, is proposed. The new method is based on an analytical representation of the Huygens–Fresnel integral through a complex Fresnel integral. It yields results in the same time or even faster than the method based on the Fourier transform and is simpler and more stable.

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INTRODUCTION

The paper examines new aspects of the theory of nanofocusing of hard synchrotron radiation beams (SR) long compound refractive lens (CRL), the basics of which are presented in [1]. A new element of the theory is the inclusion of the aperture of the long CRL together with the analytical formula for the CRL propagator [2, 3], which does not take the aperture into account. For large aperture CRLs and for relatively low SR photon energies (5–15 keV), the aperture does not affect the result, since the SR beam is completely absorbed at the edges of the aperture and the degree of focusing depends on the effective aperture, which is determined by the absorption. It has been shown previously [4, 5] that focusing to a minimum size (two tens of nanometers [6]) is possible only for CRLs with a small aperture and at high photon energies (more than 30 keV), when absorption becomes very weak. In this case, the theory without taking into account the aperture shows a greatly overestimated degree of focusing. To obtain realistic results, aperture must be taken into account.

It has been proposed to partially take into account the CRL aperture by closing the SR beam outside the aperture with a slit installed in front of the CRL [7], but this works well only in the case of very large distances from the SR source to the CRL. For third and fourth generation SR sources [8], the distances from the source to the experimental station are large, but if the CRL focuses the secondary source at the focus of another CRL, this technique will not work. The beam size at the entrance to the CRL in this case is smaller than the aperture, and the maximum beam size is inside the CRL (Fig. 1a). Problems also arise when calculating the CRL rocking curve when the beam enters the CRL at a large angle. The new version of the theory solves these problems with acceptable accuracy.

Another problem is calculating the beam size and its structure at the focal length. There are different ways to calculate the transfer of the radiation wave function through air. This problem is partly discussed in [9], where three calculation methods are compared: the Runge–Kutta method for solving differential equations; the oriented Gaussian beam method; the Huygens–Fresnel method with integral calculation using the fast Fourier transform procedure (FFT) [10]. It has been shown that the third method gives an answer many times faster than the second, while the first is completely ineffective. This conclusion, generally speaking, has been known for a long time and almost all authors use the FFT procedure for calculating coherent SR optics. But the FFT method also has problems, which are discussed in the section New method for calculating the SR wave function after CRL.

In this paper, a new calculation method is proposed, which is not universal, but is applicable for calculating the SR beam sizes after CRL. It is fast and extremely accurate. In it, the Huygens–Fresnel integral is expressed in terms of the complex Fresnel integral of a complex argument. A method for quickly calculating such an integral is proposed.

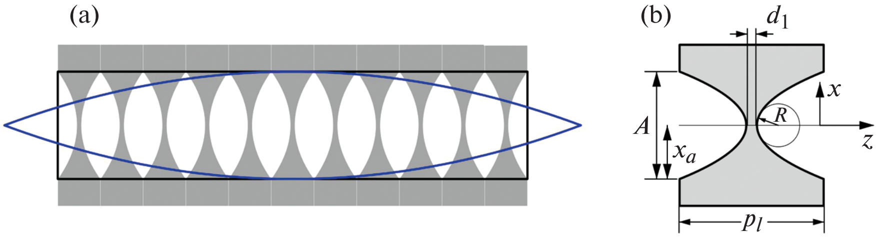

Fig. 1. General view of CRL as a periodic structure and the ray trajectory inside CRL (a). Parameters of one period, where A – aperture, $x_a = A/2$, R – radius of curvature of a parabolic surface, d_l – thickness of the thin part, p_l – the length of the period, and the coordinate axes (b).

FOUNDATIONS OF A NEW VERSION OF THE THEORY

Figure 1a shows a general view of a long CRL and highlights the focusing region, which has a height equal to the aperture A, and length $L = p_l n_l$, where p_l is the length of one period, n_l is number of periods. Figure 1b shows the main parameters of one period, including the radius of curvature of concave parabolic surfaces R and the thickness of the thinnest part d_l in the middle of the period. At the same time, $p_l = x_a^2/R + d_l$, where $x_a = A/2$. The coordinate axes used in the calculations are also shown. In the analytical theory [2, 3], the variable thickness of the material is replaced by a variable density, and the material along the axis z is considered continuous, i.e. its density does not depend on z.

For the problem in this formulation, it was possible to obtain the CRL propagator in the form $\exp(ib_0 + ib_1(x^2 + x_1^2) + ib_2xx_1)$, where x is the coordinate on the output surface of the CRL, x_1 is the coordinate on the input surface, b_0, b_1, b_2 are known complex coefficients. If the CRL is exposed to radiation from a point source with coordinates x_s and z_s, then in the paraxial approximation, the wave function is equal to the exponential whose argument is proportional x_1^2, and the integral of the product of the propagator by such a function has the form of $\exp(ia_0 + ia_1x + ia_2x^2)$ with new complex coefficients, which are calculated analytically. It is assumed that the CRL has no aperture, since it is not included in the result.

Geometric optics allows taking into account the aperture in the same approximation of a continuous medium with an inhomogeneous axis x density. It is shown that the ray trajectory inside the long CRL is described by the equation

$$x(z) = x_0\cos(z/L_c) + \theta_0 L_c \sin(z/L_c),\quad L_c = (p_l R/2\delta)^{1/2}, \tag{1}$$

where x_0 and θ_0 are initial coordinate and angle of the ray upon entering the CRL, when $z = 0$, i.e. coordinate z is counted from the beginning of the CRL. The complex refractive index of a medium is written as $n = 1 - \delta + i\beta$. For the angle between the ray and the axis z, there is also an equation

$$\theta(z) = dx/dz = \theta_0\cos(z/L_c) - (x_0/L_c)\sin(z/L_c). \tag{2}$$

Using these equations, one can calculate ray trajectories that never go beyond the aperture, but are extreme in the sense that at some point they touch the edges of the aperture.

These trajectories determine the width of the beam at the input A_0 and at the exit A_1 of CRL. The final expression for the wave function at the output of the CRL is

$$\psi_0(x) = (A_0/A_1)^{1/2}\exp(ia_0 + ia_1x + ia_2x^2) \times \theta(x_1 - |x - x_0|), \tag{3}$$

where $x_1 = A_1/2$, x_0 is the central point of the region with width A_1, $\theta(x)$ is the Heaviside function, equal to zero if $x < 0$, and one if $x > 0$. Real part of the parameter a_0 does not affect the intensity, but the imaginary part must be taken into account. The explicit form of the coefficients is written out in [1]. Wave function $\psi_1(x, z)$ at a distance z from the end of CRL is equal to the convolution $\psi_0(x)$ with Fresnel propagator

$$\psi_1(x, z) = (i\lambda z)^{-1/2}\int dx_1 \exp(i\pi[x - x_1]^2/\lambda z)\psi_0(x_1). \tag{4}$$

A new method for calculating such an integral taking into account the explicit form (3) for the function $\psi_0(x)$ is discussed in the section New method for calculating the SR wave function after CRL.

LONG CRL ROCKING CURVE

The long CRL is not only a focusing element, but also a collimating element in the sense that if a converging SR in a wide angular range is incident on it, then the SR from a smaller angular range remains at the output. Or, if there is a corner $\alpha > 0$ between the CRL axis and the axis z, then the integrated intensity of SR at the output of CRL will depend on this angle. This relationship is called a rocking curve. The rocking curve of a long CRL with a large aperture was first measured in [11] at the SR ESRF source (Grenoble, France). At that time there was no detailed theory, only primitive geometric optics was used to estimate the width of the curve. The theory appeared in [12] many years later, and its results agreed well with the result in [11]. It is shown that the rocking curve for CRL is a Gaussian function in the case when the actual aperture does not play a role due to absorption, and a formula is obtained for calculating the half-width of this function. Moreover, there is an online program [13] that calculates it together with other SR beam parameters after focusing the SR beam using CRL.

Recently, the rocking curve of a planar, nearly nanofocusing CRL was measured at the KISI-Kurchatov source (Moscow) at a photon energy of 18 keV, when the absorption is still high [14]. The results again agreed with the theory without taking the aperture into account. A new program for calculating the rocking curve taking into account the aperture was created as part of the universal XRWP program [15]. Let's look at an example of using this program for a case when the aperture significantly affects the result. Let the CRL parameters correspond to the manufactured lens [16] with an aperture of A = 30 μm. This CRL has the following parameters: p_l = 62 μm, d_l = 2 μm, R = 3.75 μm. Let the photon energy be 50 keV (λ = 0.0248 nm), the CRL has 400 elements, and the distance to the source z_s = 13 m.

In this case, the CRL length is L = 2.48 cm, L_c = 2.46 cm. Since the angles are small, the tangent is equal to its argument with great accuracy. Calculation taking into account pure geometry without refraction of rays gives the maximum angle of ray deflection $\alpha_m = A/L$ = 1.21 mrad. Accordingly, the maximum displacement of the source is equal to $x_{sm} = z_s A/L$ = 15.7 mm. The angular transmission region of the long CRL is 2 times larger, i.e. $\Delta\alpha_g$ = 2.42 mrad. The online program [13] gives the half-width of the Gaussian function for this case $\Delta\alpha_{op}$ = 2.13 mrad. This is slightly less, but it is necessary to take into account that this is the width at half the height; the maximum width is significantly greater due to the fact that the effective aperture is larger than the real aperture due to absorption.

Figure 2 shows the rocking curve for the case under consideration, calculated using the formulas of the new theory. The integrated intensity is measured in micrometers because it is the product of the average relative intensity and the beam width in micrometers. In fact, this is the effective aperture defined in [17]. The new rocking curve does not have the shape of a Gaussian function, especially in the lower part. Its half-width is 1.42 mrad, and its full width is 2.2 mrad. That is, the online program in this case significantly overestimates the width of the rocking curve. The presence of sharp aperture edges and the use of geometric optics approximation for CRL lead to a sharp decrease in the effective aperture to zero at angles greater than 1.1 mrad. The maximum angle turned out

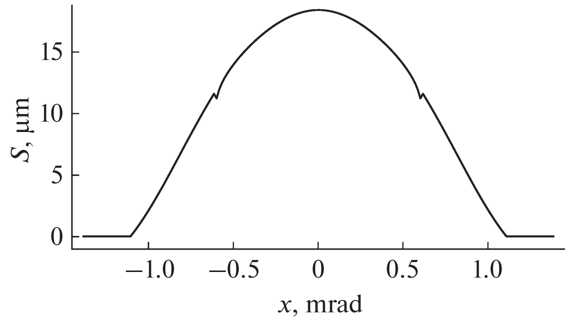

Fig. 2. Rocking curve of CRL at A = 30 μm, p_l = 62 μm, d_l = 2 μm, R = 3.75 μm, n_l = 400, photon energy 50 keV and distance z_0 = 13 m.

to be slightly smaller than would follow from the formal ray trajectory.

The calculation was carried out for a point source. The real source has transverse dimensions, so the curve must be averaged over the angular size of the source. With a source size of 100 μm and a distance of 13 m, this size is equal to 0.008 mrad. This is much less than the half-width of the rocking curve. It is obvious that the width of the rocking curve depends on the distance between the source and the CRL. Such a curve can also be calculated for small distances, but this is beyond the scope of this study.

In Fig. 2, a slight discontinuity in the curve can be seen. This failure is associated with anomalous behavior of trajectories when one of them touches the edge of the exit aperture. When the source point is shifted by 8 mm (angle is 0.615 mrad), the left trajectory reaches the edge of the aperture, and the right one is still approximately 5 μm from the center and also on the left. In this case, the maximum of the curve is 1.394, the half-width (almost equal to the width) is 9.465 μm, the integral is 11.583 μm. With a displacement of 7.8 mm, the analogous numbers are 1.409, 9.413, 11.206. Although the maximum is larger, the half-width is smaller, i.e. the left trajectory does not bend as much. And with an offset of 8.2 mm, the following parameters were obtained: 1.378, 9.365, 11.235. In this case, the left edge does not shift, but the right edge shifts to the left, reducing the beam width, and such dynamics occur with further shift of the source. Experimental detection of this feature may have practical significance.

A NEW METHOD FOR CALCULATING THE SR WAVE FUNCTION AFTER CRL

The standard method for calculating the convolution of two functions is the Fourier transform method using the FFT procedure. This procedure makes the calculation very fast, but the correct answer is obtained only if certain conditions are met. For the Fourier transform, a grid of points with a step d and the number of points n is used. The result in reciprocal space is obtained on a grid with the same number of points n and step $D = 2\pi/and$. Since the Fourier integral is calculated over infinite limits, the integrand must be equal to zero, together with all derivatives, at the edges of a region of size *and* in direct space and nD in reciprocal space.

The complications this leads to can be shown using the example of the Gaussian function. It is known that the Gaussian function has the same form in direct and reciprocal spaces, only the half-widths of these functions in direct w and vice versa W spaces are related by the relation $wW = 5.55$, while the product of the grid steps satisfies the relation $dD = 6.28/n$, i.e. it depends on n. To represent a function equally well in both spaces, one must take $d = w/m$ and $D = W/m$. In this case, it is necessary that the following relation be satisfied: $n = 1.13\ m^2$. But then the calculated regions in both spaces are obtained in m times greater than the half-widths of the functions themselves.

For calculating the convolution with the Fresnel propagator, the situation is more complicated, since the beam size at the focus can be 1000 times smaller than the aperture size, and even in the approximation where only 10 points are reserved for the peak half-width, the total number of grid points must be more than 10,000, and in this case, a lot of points will simply contain zeros. On the other hand, at other distances, i.e. not in focus, the beam size is relatively large, but the Fresnel propagator oscillates very strongly in reciprocal space, especially at large distances. That is, in order to have a step in reciprocal space smaller than the oscillation period, it is necessary to take a large size of the calculation domain in direct space. It is not always possible to calculate the result for all distances using the same grid of points. However, with the correct choice of parameters, the result can be obtained.

In this paper, to calculate the SR beam intensity curve after CRL focusing, it is proposed to use a method that has not been used anywhere yet, namely, to use the complex Fresnel integral (**CFI**):

$$F(x) = x\int ds\theta(s[1-s])\exp(i(\pi/2)x^2s^2). \quad (5)$$

Substituting (3) into (4), we obtain the integral in the form $\psi_1(x, z) = C(x, z)T(x, z)$, where

$$T(x,z) = \int dx_1 \exp(-i\beta x_1 + i\gamma x_1^2) \times \theta([x_1 - x_b][x_e - x_1]). \quad (6)$$

Here x_b and x_e are the lower and upper boundaries of the region of width A_1, i.e. the boundaries at which the beam leaves the CRL; $\beta = 2gx - a_1$, $\gamma = g + a_2$, $g = \pi/\lambda z$,

$$C(x,z) = (gA_0/i\pi A_1)^{1/2}\exp(i[a_0 + gx^2]). \quad (7)$$

The integral in (6) can be expressed in terms of CFI (5) as follows:

$$T(x,z) = A\exp(-i\gamma B^2)[F([x_e - B]/A) - F([x_b - B]/A)], \quad (8)$$

where $A = (2\gamma/\pi)^{-1/2}$, $B = \beta/2\gamma$.

For a real argument, CFI is calculated very quickly using simple formulas with coefficients chosen in such a way that the answer is very close to the real answer. But in this case, the argument x in (5) complex. It is necessary to use formulas that allow analytical continuation into the complex plane. Coefficients a_1 and a_2, if we take into account the absorption of SR in CRL, are complex. The specificity of the problem is that the imaginary parts of these coefficients are significantly smaller than the real ones, i.e. the exit into the complex plane occurs over a small distance. For this reason, when analyzing the accuracy of calculations, it is sufficient to consider only the real part.

For small values x to calculate the function $F(x)$ one can use a power series

$$F(x) = \sum_{k=0}^{\infty}\frac{(\pi i)^k x^{(2k+1)}}{2^k(2k+1)k!} \quad (9)$$

Generally speaking, the series converges for any values x, but a few terms of the series are sufficient only for small values. For large values, an asymptotic series can be used

$$F(x) = (1+i)/2 + \exp(i\pi x^2/2)(i\pi x)^{-1}[1 + (i\pi x^2)^{-1}] \quad (10)$$

For the real argument, formulas (9) and (10) give approximately the same values at $x = x_0 = 4.7$. That is, when $x_r < x_0$ it is necessary to carry out calculations according to formula (9), and when $x_r > x_0$ – according to formula (10). Here x_r is real part of x. The advantage of this calculation method is that the grid of points is used only to calculate the final result. It can have an arbitrary step and an arbitrary number of points.

There is only one problem. For CRL, parameter $a_{2r} < 0$. Focal length z_f is determined from the condition $\gamma_r = 0$. At $z > z_f$ we get $\gamma_r < 0$, and parameter A receives a large imaginary part, which leads to an incorrect result if calculated using formula (8). The problem is solved as follows. In (6), it is clear that if we change the signs of the parameters simultaneously β_r and γ_r, then we obtain the complex conjugate value of the integral. This is exactly how it should be done $z > z_f$, i.e. change the signs, perform the calculation and then take the complex conjugate value. This method allows one to calculate the SR wave function at arbitrary distances z, including even very large ones.

A new method for calculating the wave function at an arbitrary distance after the CRL is implemented in the XRWP program [15] simultaneously with a new calculation method at the end of the CRL that takes the aperture into account. It received the number 6,

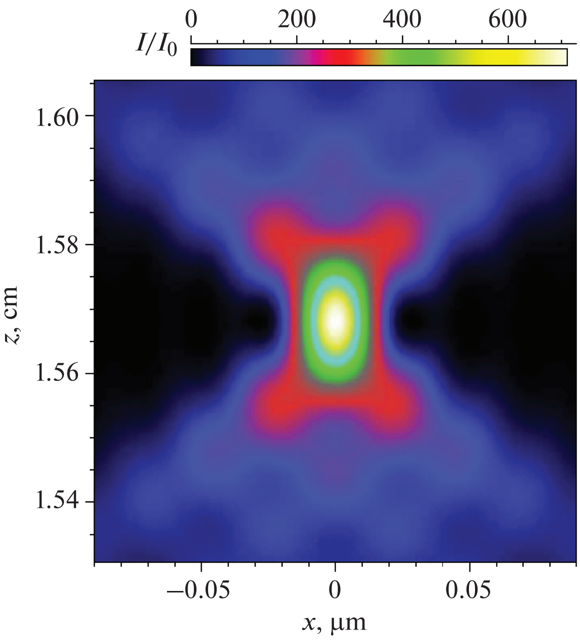

Fig. 3. Distribution of the relative radiation intensity in the focal region for the CRL parameters indicated in the caption to Fig. 2, calculated using method 6 of the XRWP program [15].

and the method of calculating the distance through the FFT procedure simultaneously with the new calculation method at the end of the CRL – number 5. For the 30 μm aperture CRL presented in the previous section, the focal length measured from the end of the CRL is $z_f = 1.5656$ cm. Since at this distance the half-width of the SR beam is 24 nm, then in method 5 the grid step is d taken equal to 1 nm, and the number of points $n = 2^{16} = 16 \times 1024$. In this case, the size of the computational domain was only slightly larger than the size of the SR beam at the output of the CRL and smaller than the CRL aperture. With fewer points, the result was incorrect. After calculation, the result was interpolated onto a grid of points with a step d_1 = 0.25 nm and the number of dots n_1 = 301. In method 6, the calculation was carried out directly on a grid of points with d_1 and n_1. A square matrix was calculated $I/I_0(x,\ z)$ on the axis interval z from 1.5306 to 1.6056 cm. The calculation result using method 6 is shown in Fig. 3.

Calculation using method 5 gave exactly the same picture. In this case, the value at the maximum of the relative intensity was equal to 728 instead of the more accurate value of 729. That is, there is almost no difference between the FFT method and the new CFI-based method. As for the matrix calculation time, on the computer used it took 5 s for method 6 and only 3.5 s for method 5. But if we take the number of points on the axis x not 301, but 151, then the calculation time for method 5 will not change at all, and for method 6, the time will be halved with practically the same result. In addition, there is the possibility to optimize the speed of CFI calculation in the future, as well as formula (8). The new method is also good because it is psychologically more comfortable, since only what is needed is calculated and nothing unnecessary.

CONCLUSIONS

For the first time, the rocking curve of a long CRL has been calculated within the framework of a new version of the theory of nanofocusing of SR beams using a long CRL, i.e., taking into account the aperture based on geometric optics, consistent with the long CRL propagator obtained in [2, 3] more than 20 years ago. A computer program for such calculations has been developed within the framework of the general XRWP program [15] for solving a wide range of SR optics problems. A new method for calculating the SR wave function after a long CRL is proposed and implemented based on the calculation of the complex Fresnel integral of a complex argument. The new method is in some cases the fastest compared to other methods, including the FFT-based method.

The theoretical results obtained will enable successful prediction and analysis of experimental data on new fourth-generation SR sources, which will be created in Russia in the near future. A more detailed analysis of focusing using long cascaded CRLs, in which the aperture is variable, will be made in the future.

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CONFLICT OF INTEREST

The author of this work declares that he has no conflicts of interest.

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