A HIGH-ACCURACY METHOD OF COMPUTATION OF X-RAY WAVES PROPAGATION THROUGH AN OPTICAL SYSTEM CONSISTING OF MANY LENSES

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Abstract: The propagation of X-ray waves through an optical system consisting of many X-ray refractive lenses is considered. Two differential equations are contemplated for solving the problem for electromagnetic wave propagation: first – an equation for the electric field, second – an equation derived for a complex phase of an electric field. Both equations are solved by the use of a finite-difference method. The simulation error is estimated mathematically and investigated. The presented results for equations show that in order to establish a high accuracy computation a much smaller number of points is needed to solve the problem of X-ray waves propagation through a multi-lens system when the method for the second equation is used. The reason for such a result is that the electric field of a wave after passing through many lenses is a quickly oscillating function of coordinates, while the electric field phase is a quickly increasing, but not oscillating function. Therefore, a very detailed difference grid, which is necessary to approximate the considered electric field can be replaced by not such a detailed grid, when computations are made for the complex wave of the electric field. The simulation error of both suggested methods is estimated. It is shown that the derived equation for a phase function allows efficient simulation of propagation of X-rays for the multi-lens optical system.

Keywords: X-ray wave, X-ray optic, lens, non-uniform medium, focusing, numerical method, simulation, finite-difference, stability, numerical error, wave phase, electromagnetic wave, fast oscillating function

1. Introduction

The X-ray microscopy, a new method to examine internal structures of microobjects has been actively developed during the last 20 years. Application of biconcave lenses made of light metals is one of the most perspective ways of

focusing of X-ray beams [1–3]. Such lenses focus X-ray beams because the phase propagation velocity of X-ray waves in light metals exceeds slightly the speed of light. This is a consequence of the form of the complex refraction index of the material $n = 1 - \delta + i\beta$, where $\delta > 0$. For example, for aluminum when photon energy is equal to 25 keV, $\delta = 8.643 \cdot 10^{-7}$, $\beta = 1.748 \cdot 10^{-9}$ [3]. The imaginary part of n defines an absorption factor. When an X-ray wave propagates through the lenses, the wave's phase is changed. The wave phase change is much larger for waves propagated near the lens aperture edges than for waves propagated near the general optic axis. It leads to an effect of focusing of X-ray waves by lenses.

Recently, beryllium has been considered as one of the most prospective materials for manufacturing lenses because this metal possesses low absorbing properties and a comparatively large refraction factor. However, lenses are manufactured from other materials as well: for example, from aluminum. In [4, 5], lenses made of glass-graphite are suggested and applied. In [6], silicon lenses have been investigated. Some lenses have been made also of boron carbide, pyrographite, teflon [7].

Modern X-ray lenses have a parabolic shape of their concave surfaces. Owing to such a form it is possible to eliminate aberrations inherent to lenses with spherical concave surfaces.

Since the refraction factor is small, the effect of focusing of one lens is weak, and often a system of many lenses is applied in order to achieve an essential effect of focusing. If lenses are arranged in a row, one after another, the lens system acts as a lens, and we are speaking about a compound refractive lens (CRL). The focal distance of one lens is given by the formula $F_1 = \frac{R}{2\delta}$, where R is a radius of curvature of a parabolic lens surface [5, 3]. For a CRL consisting of N identical lenses, the focal distance F is approximately equal to $\frac{F_1}{N}$.

The refraction index n of materials essentially depends on the frequency within the range of high-frequency electromagnetic waves. Therefore, the monochromatic, coherent source of X-ray waves is necessary to get the qualitative image with a great enlargement factor. With this aim, synchrotrons supplemented with ondulators are actively used as sources of X-ray waves.

Obtaining a high-quality image and achieving a high enlargement factor are some most important goals of the development of X-ray optics. As a consequence, now the question of the effect of defects of various lens on the image quality is topical. When we say defects, we mean any imperfections in the lens form, errors in the adjustment of lenses along the general optical axis of a system of lenses, and we also have in mind any possible internal microscopic defects: cavities, inclusions of oxides in the lens material.

This paper is devoted to the theory of numerical modeling of X-ray waves propagation in an optical system. The demands on the numerical simulation method essentially depend on our intentions. If one wants to explain the effects of focusing and image formation, then the coincidence of the results of computation with an experiment is obviously a criterion of correctness of our simulations.

Many perfect publications of such kind have been written up to the present time [8, 9, 2, 10, 11]. If simulations are carried out with the aim of explanation of physical effects, one can choose the numerical method parameters (the number of modes in the Fourier-method or the number of mesh points in the mesh method) experimentally, basing on the requirement of best agreement of the computed results with an experiment.

If one uses numerical simulation for scientific and engineering research (for example, to investigate the effect of defects on focusing and imaging), the requirements for the theoretical validity of numerical methods are higher. We often apply numerical simulations in cases when real experiments are difficult or impossible to carry out. Especially in these cases, we want to have some means of control of the simulation reliability and the available accuracy.

Moreover, even if the comparison with the experiment is possible, we have to bear in mind that the actual lens parameters are known only approximately. Also the real X-ray source is incoherent and is known only approximately. Therefore, the comparison with the experiment is not always possible to check simulations. Under these conditions, the validation of simulations can be based only on the mathematical error estimate. These mathematical tools to validate accuracy need to be developed and explored. The need to control the simulation accuracy may lead to replacement of previously developed methods with new ones, for which the accuracy is easier to control.

The computational complexity dependence on the optical system and on the experiment scheme is also an important issue. Normally the paraxial Equation (1) describes the X-ray wave propagation. We shall show that when the X-ray wave passes through a system of many lenses, the solution of this equation is a rapidly oscillating function of distance from the main optical axis. Moreover, the oscillation frequency of the wave field increases exponentially with the number of lenses. The higher the oscillation frequency, the more detailed mesh is required to digitize such a function, and the greater computations are required. Therefore, although the simulations for a small number of lenses may seem quite simple, the computational complexity increases rapidly with the number of lenses, and the simulation for many lenses may be an extremely complicated computational problem. Given the computer power, one can specify how many lenses are sufficient for the computer's performance to be sufficient to perform simulations with a reasonable accuracy on the basis of Equation (1).

In case of many lenses, the computational complexity is also strongly dependent on the width of the X-ray beam incident on the lens.

In order to establish an acceptable accuracy of computations for the use of many lenses, we have proposed solving the equation for the complex phase $\Psi(x,y,z)$ of the wave instead of solving the paraxial Equation (3) for the electric field $A(x,y,z) = e^{i\Psi(x,y,z)}$. The phase function $\Psi(x,y,z)$ is not a fast oscillating function, and therefore it does not require a detailed mesh for its digitizing. The computational complexity of simulations with the Equation (9) for the phase

function does not depend on the number of lenses, and one can easily achieve a high accuracy of numerical simulations for many lenses. An electric field may be elementarily restored, when the complex phase function is a known function.

The plan of this paper is as follows. To begin with, we develop a numerical finite-difference method, which enables solving the problem of focusing of X-ray waves by 33 aluminum lenses. We investigate how detailed the difference grid should be to ensure high-quality of computation of the X-ray wave propagation through a system of 33 aluminum lenses and to ensure high quality computation of focusing of waves.

Then, we derive the Equation (9) for the complex phase $\Psi(x,y,z)$ wave. We performed calculations with the help of Equation (9) for the complex phase and we investigated the method accuracy and demonstrated the advantages of the method for the problem of X-ray wave focusing by 30 beryllium lenses. The simulation method is a particularly advantageous one when we consider the case of many lenses. As an extreme example, we performed a simulation of X-ray wave focusing by a system of 160 lenses.

In this paper, we have not taken into account incoherencies of the source of X-ray radiation, although, of course, the incoherence of the source of waves affects the focusing and imaging. We investigate the quality of approximate mathematical methods of simulation of X-ray wave propagation, but it does not depend on the source X-ray waves.

2. Main equations

2.1. Equation of propagation of a monocromatic electromagnetic wave in air

The propagation of a monochromatic electromagnetic wave of the X-ray range in vacuum (in air) has been considered in [3, 8, 2, 11]. In particular, on the basis of Maxwell's equations, the authors have shown that the equation

$$\frac{\partial A_{\text{air}}}{\partial x} = \frac{ic}{2\omega_0}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) A_{\text{air}} \tag{1}$$

describes propagation of a monochromatic electromagnetic wave of frequency ω_0 in empty space within a paraxial approach. Here c is the speed of light. The axis x is designated along the direction of propagation of the quasi-plane wave; the axes y, z are perpendicular to the x-axis. The electric field $E(x,y,z,t)$ is expressed via $A(x,y,z)$ as follows: $E(x,y,z,t) = A(x,y,z)\cdot e^{i(k_x x-\omega_0 t)}$, $k_x = \frac{\omega_0}{c}$; we take a real part of the expression. Since the connection of the electric field $E(x,y,z,t)$ with the function $A(x,y,z)$ is very simple, we sometimes call the function $A(x,y,z)$ an electric field.

Equation (1) was first proposed by Leontovich M. A. [12] in 1944 to describe the propagation of a monochromatic electromagnetic wave within the paraxial approach, and as a result, the approximate Equation (1) is often called a paraxial equation. This equation is widely used not only in the X-ray optics, but also in standard optics, in the theory of propagation of radio waves, in acoustics [13].

Equation (1) is also often called a parabolic equation due to external similarity of this equation with the heat equation, even despite the fact that the equation contains an imaginary unit in coefficients and, strictly speaking, it is not an equation of a parabolic type.

2.2. Equation of propagation of a monochromatic electromagnetic wave in a lens material or in a sample

Theoretical papers [3, 8, 2, 11] are devoted to the problems of propagation of a monochromatic electromagnetic wave with the frequency of the X-ray range in the lens material. On the basis of Maxwell's equations for a medium with a complex dielectric constant, which depends on the frequency, the authors have shown that the propagation of a monochromatic electromagnetic wave with frequency ω_0 in a lens material is well described within the paraxial approach by the equation

$$\frac{\partial A_{\text{Linz}}}{\partial x} + \frac{\omega_0}{c}[i\delta + \beta] A_{\text{Linz}} = \frac{i\,c}{2\omega_0}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) A_{\text{Linz}} \tag{2}$$

Here, as before, axis x is designated along the direction of the quasi-plane wave propagation, and axes y, z are perpendicular to axis x, δ and β denote the real and imaginary parts of the refraction index $n = 1 - \delta + i\beta$.

2.3. General equation of propagation of monochromatic X-ray waves in a non-uniform medium

It is well known that X-ray waves penetrate through practically any material and propagate practically without reflection and absorption. Therefore, the boundary condition of continuity of the function A on the border between various media is quite acceptable and widely applied [3, 8, 2, 11]. It gives us foundations to unite both Equations (1) and (2) into one general equation [14]:

$$\frac{\partial A}{\partial x} + b(x,y,z)\, A = \frac{i\,c}{2\omega_0}\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) A \tag{3}$$

Here $b(x,y,z)$ is a complex function of coordinates depending on the material:

$$b(x,y,z) = \begin{cases} 0 & \text{for air} \\ \frac{\omega_0}{c}[i\delta + \beta] & \text{for lens material} \end{cases} \tag{4}$$

Equation (3) is very convenient because it allows us to carry out calculations when we solve the problem of X-ray wave propagation through a system of lenses and also the problem of focusing and imaging. This equation allows us easily to take into account any inclusions in the lens material or other lens defects. Equation (3) also can be used to describe the X-ray wave propagation through a sample. Therefore, Equation (3) is a general equation, which is worth insightful discussion and examination.

3. Numerical simulation of propagation of X-ray waves through a system of lens and X-ray beam focusing

Basing on Equation (3), we will solve the problem of propagation of X-ray waves through a system of lenses and focusing of the X-ray beam. There are several methods of solving the problem of X-ray wave propagation through a system of many lenses. For example, in [3], a resourceful method based on replacement of a system of lenses with one long lens with an average refraction index has been developed and applied. Also, some approximate solution may be obtained by consequent combining of solutions of Equation (2) without the refraction term with solutions of the Equation (1) [11]. All these approaches are noteworthy, but they are not rigorous, whereas we try to develop rigorous methods and to get accurate estimates of accuracy of methods.

We intend to solve Equation (3) numerically, with the help of the finite-difference methods, and we consider Equation (3) in the parallelepiped Ω with a sufficiently large size. This parallelepiped includes all lenses by supposition.

We denote by $\partial\Omega$ the boundary of the parallelepiped, which is intersected by the y, z axes. We denote by S the square which is the intersection of the parallelepiped with the plane Oyz. Within the square S, we define a difference mesh with the nodes (y_n, z_m) and with a constant step h along axes y, z.

The finite-difference methods may not by the most efficient, but they are very flexible and universal, and they are good for obtaining general information about the solution's behavior.

We approximate Equation (3) by the following system of ordinary differential equations

$$\frac{\partial A_{n,m}}{\partial x} + b(x, y_n, z_m) A_{n,m} = \frac{ic}{2\omega_0} \left(\frac{A_{n+1,m} - 2A_{n,m} + A_{n-1,m}}{h^2} + \frac{A_{n,m+1} - 2A_{n,m} + A_{n,m+1}}{h^2} \right) \tag{5}$$

We impose a natural boundary condition $A_{n,m}\big|_{\partial\Omega} = 0$ on the border $\partial\Omega$.

The system of ordinary differential Equations (5) can be solved with the use of any standard numerical method, which enables solving a system of ordinary differential equations; for example, we can apply the Runge-Kutta method of the second order of accuracy.

The stability and convergence of the suggested method has been proved in [14].

3.1. Estimation of accuracy of numerical simulation

It is well known that the accuracy of finite-difference simulations can be found out by comparing the computations made in various steps of the difference mesh.

Table 1. Test simulation parameters

number of aluminum lenses	$N = 33$
lens curvature radius	$R = 0.2\,\text{mm}$
energy	$15\,\text{keV}$
ω_0	$7.254 \cdot \pi \cdot 10^{18}\,\text{s}^{-1}$
δ	$2.414 \cdot 10^{-6}$
β	$1.299 \cdot 10^{-8}$

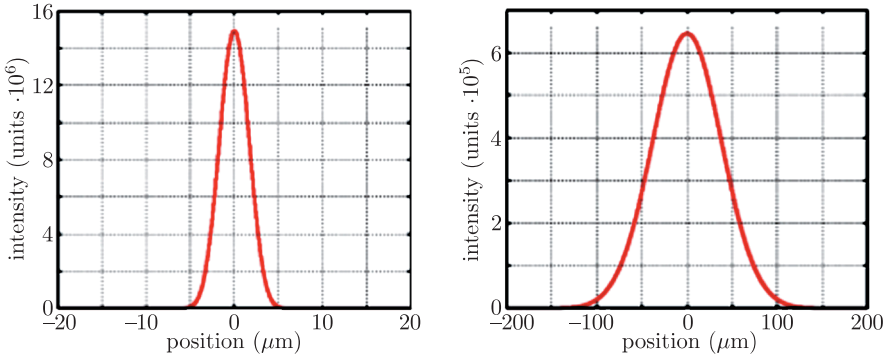

Figure 1. Results of hard X-ray focusing with 33 perfect aluminum lenses immediately after the lenses (right), and at a distance of 1.298 m from the lens (left) with FWHM = 3.92 μm, and focal distance = 1.2470340 m

We provided a computation of X-ray propagation and X-ray focusing and we found parameters of a focal spot for the optical system with parameters given in Table 1.

The results of simulations of X-ray propagation through one-dimensional lenses, which depend on the number of nodes and a grid step h are shown in Table 2.

Table 2. Results of computation of the focal distance and FWHM for different values of h.

	number of points	h	FWHM	focal distance
1	40 000	0.000000025	3.95 μm	1.2480707 m
2	50 000	0.00000002	3.92 μm	1.2470340 m

We want to estimate the numerical solution error. The Runge rule [15] of practical estimation of the numerical computations error is well known in the numerical methods theory. For the first time the Runge rule was formulated for approximate computation of integrals, but this rule is applicable also to estimate the accuracy of other quantities. The electric field depends on coordinates, but the Runge rule is applied for estimation of the accuracy of quantities which are independent from coordinates. The focal length and the FWHM (full width at half magnitude) are important characteristics of an optical system.

In the classical variant of the Runge rule, the computations carried out with a fixed step and a double step are used. In our case, the steps in both cases of computations are not very different. Therefore, we generalize the classical Runge rule to a more general case, when the steps are different, but not necessarily equal to h and $h/2$.

3.1.1. Modified Runge rule and its application for evaluation of errors of numerical simulations

Let us compute the Z value approximately, and let Z_{h_1} and Z_{h_2} be the results of approximate computations performed with steps h_1 and h_2, respectively ($h_2 < h_1$), and let the main error term Q have a structure of $Q = C * h^k$, where h is a step, C is a constant, and k denotes the accuracy order of the method. Then, it is easy to show that

$$Q = \left| \frac{Z_{h_1} - Z_{h_2}}{\left(\frac{h_2}{h_1}\right)^k - 1} \right| \tag{6}$$

The numerical method (5) is a method of the second order of accuracy, therefore we have to take $k = 2$ in (6). We apply the Runge rule (6) to the results of computations in Table 3 and we find that the error of computation of the FWHM is approximately 1% and the error of computation of the focal length is 0.2%. That is, for $N = 40\,000$, the simulation accuracy is acceptable, but it is not very high. The focal length for the optical system as described in the Table is computed more accurately than the FWHM.

Therefore, we have come to the outcome that one needs to use about 40 000 points of a difference mesh along each axis in order to compute reliably the parameters of the focal spot with two significant figures. It also means that the high-accuracy simulations of propagation of an electromagnetic wave through a system of 33 two-dimensional aluminum lenses require that a supercomputer is used.

3.2. Discussion and explanation of simulation results

In this section we want to understand why a very detailed mesh is necessary to guarantee precise simulations. Is it a feature of the applied finite-difference method, or maybe some complicated behavior of the wave exists which compels to use a very detailed mesh?

We shall see below that a detailed mesh is needed due to the behavior of the wave which passes through many lenses.

The right-hand-side term of Equation (3) is comparatively small [9, 11]. If we neglect this small right-hand term, we obtain an approximate formula (7) for the function $A\ (x,y,z)$. This formula approximately describes the behavior of the wave field $A\ (x,y,z)$, which passes through a system of N lenses [9, 11]:

$$A(x,y,z) \approx A(0,y,z)e^{i\phi(y,z)} \qquad \phi(y,z) = \frac{\left(y^2+z^2\right)}{l^2} \tag{7}$$

where $l^2 = \frac{cR}{\omega_0 \delta N}$, R is a radius of curvature of parabolic lenses and N denotes the number of lenses. Here $A(0,y,z)$ is the electric field before the lenses. In the calculations, we used the function $A(0,y,z) = \exp\left(-\frac{y^2+z^2}{2\sigma^2}\right)$, $\sigma = 50\,\mu$m. For simplicity, we have put $\beta = 0$, though consideration of attenuation is not difficult, but taking attenuation into account it is not important for our estimates.

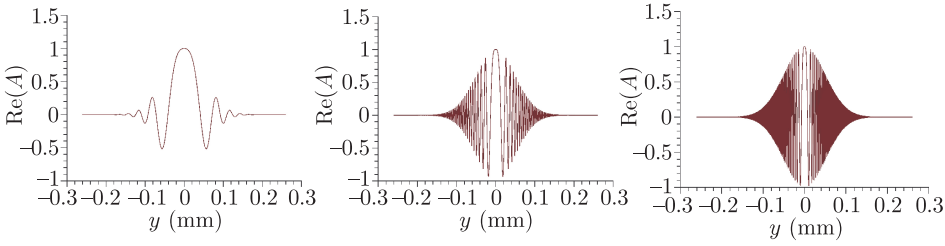

Figure 2. Field $\Re(A)$ immediately after the wave passed through one lens, a system of 10 lenses and a system of 33 lenses; the computations are made with the formula (7).

When we use many lenses, and the frequency is high and the curvature of lenses is small, then the denominator l^2 is small. For an optical system of 33 aluminum lenses and energy of X-ray waves 15 keV, $l \approx 6 \cdot 10^{-6}$ m.

It is obvious that in numerical simulations phase ϕ in (7) has to be varied insignificantly at one step h of the difference mesh. This means that the conditions $\left|\frac{\partial\phi}{\partial z}h\right| \ll 1$, $\left|\frac{\partial\phi}{\partial y}h\right| \ll 1$ should be satisfied. If we take the lens aperture d into consideration, we obtain the condition $h \ll l^2 \approx 10^{-7}$ m that is comparable with h presented in Table 2.

The phase ϕ becomes a faster and faster growing function, when the wave passes through a system of 33 lenses. Correspondingly, the function $A(x,y,z)$ becomes an increasingly faster oscillating function, when the wave passes through the system of 33 lenses, and therefore, we are compelled to use a very detailed difference mesh for digitizing such a function. The field $\Re(A)$ for the waves, which passes through systems of one-dimensional lenses, depends on the number of lenses in the system, which is shown in Figure 2. The charts clearly explain why a very detailed mesh is needed in the case of many lenses. Obviously, a very detailed mesh is required in order to digitize the behavior of the fast oscillating function, but it is not caused by any peculiarities of the applied mathematical methods.

4. Equation for a phase-function instead of equation for an electric field as a technology of accurate simulations

In the investigated problem of wave propagation through lenses, the refraction term is not large, but nevertheless accurate consideration of the contribution of this term is necessary.

The approximate solution (7) shows that it is expedient to change the dependent variable in Equation (3) and to search for a solution of Equation (8) in the form:

$$A(x,y,z) = e^{i\Phi(x,y,z)} \tag{8}$$

The suggested replacement of the dependent variable is expedient because while the function $A(x,y,z)$ is quickly oscillating, the phase-function $\Phi(x,y,z)$ is a usual, large-valued, but non-oscillating function. Therefore, if we simulate the behavior of the phase-function $\Phi(x,y,z)$, then the necessary difference grid requirements are essentially lower, and we can easily reach high accuracy of computation of Φ. Then one can easily calculate the electric field $A(x,y,z)$ by means of the formula (8).

The function $A(x,y,z)$ is defined unequivocally, if we know $\Phi(x,y,z)$. However, the $\Phi(x,y,z)$ is defined by $A(x,y,z)$ ambiguously. Fortunately, we have a priori information about the initial function $\Phi(0,y,z)$: the incident X-ray wave before the lenses has a phase being approximately constant and slowly dependent on the coordinates. It fully determines the correctness of the statement of condition $\Phi(0,y,z)$.

The equation for $\Phi(x,y,z)$ is derived elementarily and has the following form:

$$\frac{\partial\Phi(x,y,z)}{\partial x} - ib(x,y,z) = \frac{c}{2\omega_0}\left[i\left(\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Phi(x,y,z) - \left(\frac{\partial\Phi(x,y,z)}{\partial y}\right)^2 - \left(\frac{\partial\Phi(x,y,z)}{\partial z}\right)^2\right] \tag{9}$$

We suggest using this equation instead of Equation (3) for simulations of propagation of a monochromatic X-ray wave through a system of lenses.

Due to the reasons described above, Equation (9) allows providing easily high-accuracy computation of X-ray wave propagation through a system of lenses. This equation is especially productive in the case of many lenses.

If the experiment scheme is such that a sample is located before the system of lenses, then Equation (9) also has to be used for simulation of propagation of X-ray waves through the sample.

The Equation (9) is widely known; it was first proposed by Rytov S. M. in 1937, when he considered the diffraction of light on ultrasonic waves. In Rytov's theory [16], the supposition that the medium parameters are slowly changing with coordinates has been used for derivation of an equation in the form (9). During our derivation of the Equation (9), the assumption of slow variation of medium parameters was not required, and the Equation (9) follows directly from Equation (3). Weakening of the requirements apparently has become possible due to the high penetration capability of X-ray waves, which leads to a slow change of wave parameters even when medium parameters are changed abruptly.

Rytov S. M. has developed a perturbation theory for solution of the Equation (9), the method of smooth perturbations. This perturbation theory starts from the linearized equation, and the contribution of nonlinear terms is taken

into account in the following orders of the perturbation theory. Rytov's perturbation theory is hardly acceptable for solution of our problem because the nonlinear terms play a leading role in our problem of focusing. We will solve the Equation (9) with a finite-difference method, without any simplifications.

If we neglect the refractive term in (9) and if we put $b(x,y,z)=0$, then we arrive at a geometrical optic equation, written in the approximation when only the wave along the positive direction of x-axis is taken into account and when the scales of the wave along y, z axes are much larger than the scale of the wave along x-axis.

4.1. Example of calculation of wave propagation and focusing with the help of equation for a complex phase

Below we solve Equation (9) with a finite-difference method. The numerical scheme for solving the Equation (9) is similar to (5), but the nonlinear terms are taken into account. The numerical solution for the case of one-dimensional lenses has been computed for the following values of the parameters

- the number of beryllium lenses $N=30$
- the lens curvature radius is $R=50\,\mu$m
- energy of 12.4 keV ($\omega_0=6\cdot\pi\cdot10^{18}\,\mathrm{s}^{-1}$)
- $\delta=2.2156\cdot10^{-6}$, $\beta=3.1801\cdot10^{-10}$
- form of A before lenses: $A=\frac{1}{2\pi\sigma^2}\exp\left(-\frac{y^2}{2\sigma^2}\right)$, $\sigma=297\,\mu$m.

The computation results are shown in Figure 3–4. As can be seen, the real part of Φ is changing almost linearly, but still it changes extremely fast after the set of lenses.

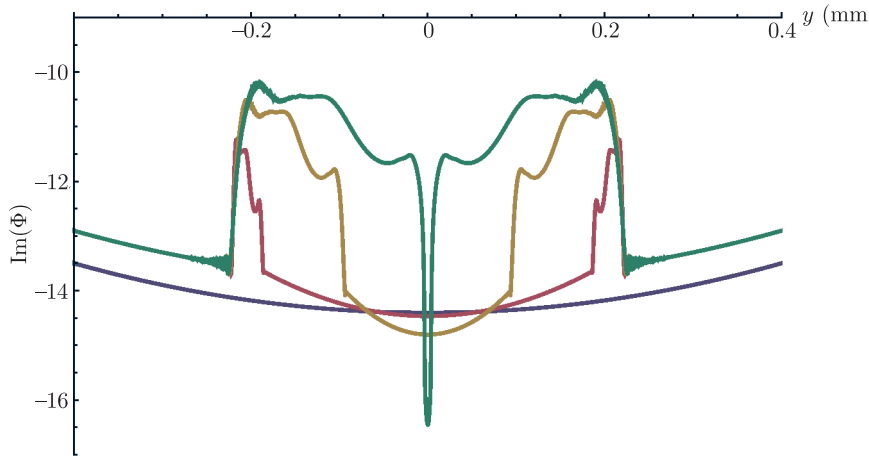

Figure 3. Imaginary part of Φ (it can be also described by $-\ln|A|$ on y). Blue – initial condition, Red – results 4 cm after set of lenses, Yellow – results 20 cm after set of lenses, Green – results 36 cm after set of lenses. Calculation provided for 4000 points.

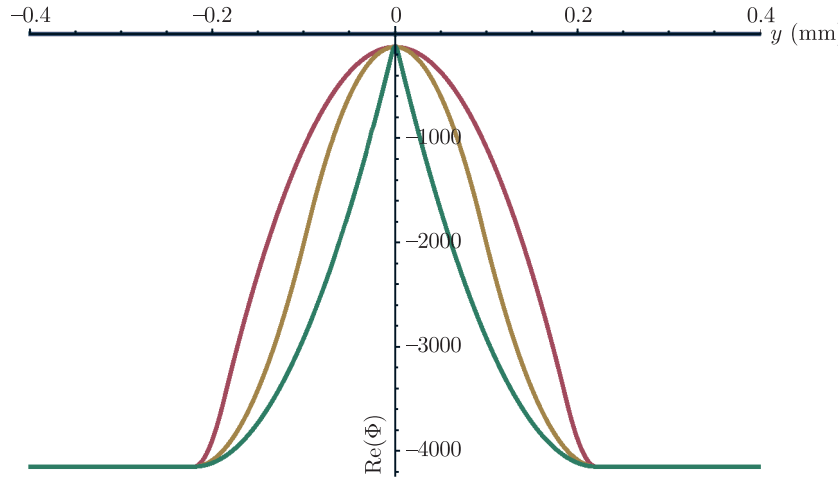

Figure 4. Real part of Φ. Blue – initial condition, Red – results 4 cm after set of lenses, Yellow – results 20 cm after set of lenses, Green – results 36 cm after set of lenses. Calculation provided for 4000 points.

4.1.1. Consideration of the complex phase method accuracy

For the investigation of the computational error, we performed simulations with 4000 points and 8000 points and we evaluated the computational error with the Runge rule (6). The results of FWHM and focal length calculations are shown in Table 3.

Table 3. Table with results obtained with numerical solution of Equation (9)

Number of points	h	FWHM at 0.34 m after CRL	focal distance
4000	0.00000025	17.3315 μm	0.36575 m
8000	0.000000125	17.3056 μm	0.365938 m

An analysis of the computational results in Table 3 showed that the computational error of the focus distance was less than 0.07%. The computational error of the FWHM at the distance of 34 cm was less than 0.2%.

Thus, using Equation (9) we achieved a high accuracy of the results, despite the fact that the mesh used in this simulation contains 10 times fewer points along each direction than in the previous case. In the case of two-dimensional lenses, the Equation (9) allows using 100 times fewer mesh points. In this sense, application of the Equation (9) is justified.

Moreover, when we integrate the equation, thanks to the use of the 10-fold step h with respect to the previous case, without any loss in accuracy we can use also the 100-fold steps along the OX-axis. Therefore, we have a 10^4-fold decrease in the number of computations.

Figure 4 shows the effect of focusing of an X-ray wave by a CRL consisting of 160 lenses; the simulation was performed using the Equation (9) for the complex phase.

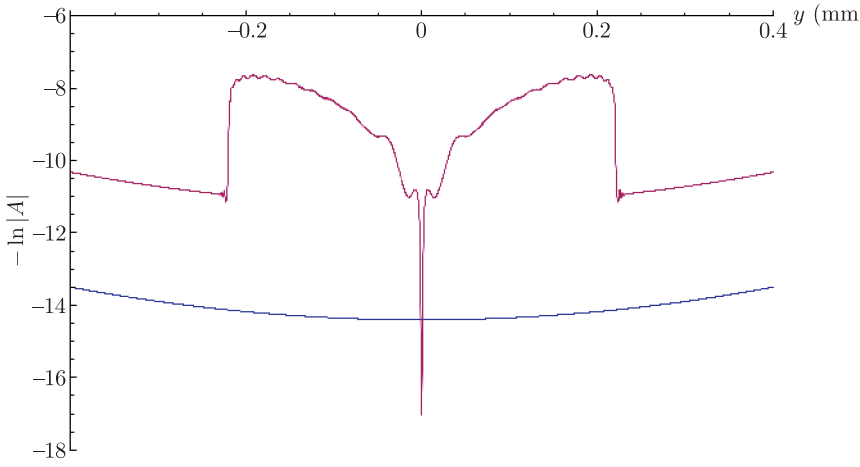

Figure 5. Imaginary part of Φ (it can be also described by $-\ln|A|$ on y). Focal spot for 160 lenses (focal distance – 7 mm after last lens). Calculation performed for 4000 points.

4.1.2. Range of applicability of the complex phase method

The focal spot size is very small, and only a small number of mesh points belong to the focal spot. Therefore, despite the fact that the parameters of the focal spot are computed with a high accuracy, the numerical simulation accuracy greatly falls at a distances where the wave passes through the focal spot.

In order to simulate complex phase changes (9) at distances greater than the focal distance method, what is described above is unadvisable and some other methods would be preferable. For example, if we are interested in distances somewhat greater than the focal distance, then we can use the symmetry of the wave field. This approach is described below in the Section 4.1.3.

When the distances under consideration are much greater than the focal distance, it is advisable to apply a numerical method based on an analytical solution of the equation (1).

4.1.3. The use of spatial symmetry

We will consider the simulation of the wave field at small distances after the focal distance. In this case, a very simple way to compute the wave field may be based on symmetry.

We begin with consideration of a system of ideal lenses. After the wave passes through a system of lenses, a focal spot is formed. It is convenient to introduce a selected point in the focal spot – the center of symmetry – which we call the focus. We define a focus position (x_f, y_f, z_f) (center of symmetry) at the point of a maximum of $\left|A(x,y,z)\right|$.

For the sake of simplicity, while the optical system which consists of ideal lenses is considered, we can suppose that $x_f = 0$, $y_f = 0$, $z_f = 0$. The point x_f, y_f, z_f is a point of central symmetry, so

$$\Phi(x,y,z) = -\Phi^*(-x,-y,-z) + a \tag{10}$$

Here a is a real constant; without loss of generality, we can take $a=0$. Near the focus-point, the condition (10) is satisfied only approximately, because on any plane $x=\text{const}$ the wave field is formed by the waves, which have passed through the focal spot, and by waves which propagate along the optical axis and were subjected to the effects of focusing. However, the amplitudes of the latter waves are very small and these waves can be neglected.

We now turn to the general case. Let us suppose that the end of the last lens coincides with the plane $x=x_L$. If the plane $x=0$ is placed directly before the lenses, then x_L is equal to the total thickness of all lenses. We define the position (x_f,y_f,z_f) of a symmetry center – the focus – as an absolute maximum of the function $\left|A(x,y,z)\right|$ at $x>x_L$. We do not assume that $z_f=0$, $y_f=0$ because the lenses may be imperfect, and the focus may be not exactly on the axis OX, but may be slightly off the OX-axis.

Moreover, in the case of imperfect lenses, the function $\left|A(x,y,z)\right|$ may have additional local maxima at some distances of the main peak. However, we assume that the deviations of lenses from an ideal are not strong, and the central symmetry approximately holds.

We denote the solution of (9) at $x_L<x<x_f$ by $\Phi_0(x,y,z)$. The function $\Phi_0(x,y,z)$ can be easily computed using the direct numerical integration of the Equation (9), and therefore we assume that it is known. Due to the central symmetry

$$\Phi(x,y,z)=-\Phi_0^*\left(2x_f-x,2y_f-y,2z_f-z\right) \tag{11}$$

Thus, we have constructed an approximate solution $\Phi(x,y,z)$ of the Equation (9) at $x\le\left(2x_f-x_L\right)$.

Considering the distances $x>\left(2x_f-x_L\right)$, it is advisable to take it into account that the linear dimensions of the image are enlarged at large distances. It is therefore advisable to calculate the enlarged image on a mesh corresponding to the size of the enlarged image. It is expedient to use the advantage that we know $\Psi(x=x_L,y,z)$ with high accuracy. The appropriate method of computation will be published somewhere else.

5. Conclusions

The paper considers simulations of propagation of monochromatic X-ray waves through a system of many lenses. We analyze the accuracy of numerical simulations and we develop high-accuracy methods.

- A general equation for the electric field with variable coefficients, allowing consideration of the problem of propagation of X-ray waves through a system of lenses is suggested as the problem of propagation of X-ray waves in an inhomogeneous medium with given properties is suggested.
- A finite-difference method for solving the general equation is developed and applied for solving the problem of propagation of X-ray waves through a system of 33 aluminum lenses.

- With the help of the Runge rules the simulation error is estimated and studied. It is shown that the mesh with about 40 000 points along each direction perpendicular to the optical axis is required for an acceptable accuracy of the approximate solution.
- The reason why a detailed mesh is necessary is analyzed. It is shown that, after the wave passes through many lenses, the wave field $A(x,y,z)$ becomes a fast oscillating function of y, z variables; the digitization of the behavior of such waves on a less detailed mesh is not possible.
- The dependence of the wave field $A(x,y,z)$ on the number of lenses is examined. When we do not use many lenses, the function $A(x,y,z)$ is not fast oscillating. However, the oscillation frequency increases exponentially with the number of lenses, making computations based on the parabolic equation difficult or impossible due to huge quantity of computations. The frequency of oscillation increases towards the aperture edges, so the computation quantity essentially depends on the width of the beam incident on the lenses.
- To circumvent the problem of the fast oscillating field and make high-accuracy simulations for many lenses possible, the equation for a complex phase is proposed. The electric field is easily calculated by a complex phase.
- The complex phase equation is solved by finite-difference methods, and advantages of the method is demonstrated. The method allows high-accuracy simulations for many lenses, despite the fact the $A(x,y,z)$ is fast oscillating in the case of many lenses.
- The proposed method has particular advantages in the case of many lenses. As an example, the focal spot of the X-ray wave, which propagates through the system of 160 lenses, is computed and shown in details.

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