

FINITE-DIFFERENCE SOLUTION OF PARABOLIC EQUATION AND NUMERICAL SIMULATION FOR X-RAY FOCUSING

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(Received 20 January 2014; revised manuscript received 10 February 2014)

Abstract: In this paper we apply the finite-difference method to solve a parabolic equation of a general problem of short wave diffraction in a conducting medium. It is based on the implicit Runge-Kutta method of the second order combined with the iterative procedure. We also present new numerical simulations for X-rays focusing using the mentioned approach. We consider CRLs with a parabolic profile with a radius of curvature up to 0.2mm. The main goal of this work is to elaborate an X-ray calculator for a PC which would present new possibilities compared to conventional ones. The correspondent code is written in FORTRAN to obtain the focal distance and diffraction spot profiles. Simulations for two cases were performed, the first one with 33 Al lenses for X-ray energy 15 keV, the results showed that we needed to consider more than 50000 points in each direction which forced us to consider a one-dimensional simulation only. For the second case we performed a simulation for several lenses, up to 15 Al lenses to perform the 2-d simulation. We have good agreement with the experimental data for the focal distance, and for the intensity at the focal plane while, for the spot size, we have smaller FWHM for the Gaussian beam at the detector than in the experimental data. We believe that the FWHM we have is smaller as our lenses are ideal without any defects.

Keywords: Finite difference model, Focusing X-rays, Runge-Kutta

1. Introduction

Most of the X-ray applications are based on their ability to penetrate materials. In materials sciences we use an electromagnetic wave with an appropriate wavelength to investigate, and examine the structure of samples. Consequently,

there is demand for focusing X-ray beams to understand biological, chemical, and physical systems. There are different ways to focus X-rays like: grazing mirrors, Fresnel plates and compound refractive lenses. In our model, as in others [1–3], we use CRLs with the parabolic profile [1] to simulate focusing X-ray beams with a diffraction account.

The article presents the results of a simulation of X-ray propagation and focusing in a frame of finite-difference approximation of a parabolic equation. The equation is derived on the basis of a standard Maxwell system for the conducting medium for an ansatz solution as a plane wave with a slow varying 3D amplitude [3], the conductivity is neglected outside the lenses. We consider the parabolic shape of lenses to focus X-rays, see e.g. [1, 2]. However, we need to mention that we use here perfect lenses without any defects. As initial condition we use Gaussian form of the beam cross-section with the coherent modulation. The general motivation for such finite-difference modeling (FDM) is, and simulations are performed, to prepare the conditions for a more complicated problem of a lens with defects. In the last chapter we will compare and discuss our results with the theoretical results and the experimental data presented in [1].

2. Problem formulation and ansatz solution

2.1. The Parabolic equation derivation

The derivation of the model equation starts from Maxwell’s system to describe the propagation in free space (before and after lenses). Inside the lenses we solve Maxwell’s equations in metals for a linear, isotropic, non-magnetic, and homogeneous medium. Thus, electric susceptibility $\chi_e(\omega_0)$, and conductivity σ will be constants. We consider also fixed frequency ω_0 , inside and outside the lenses.

We start with Maxwell’s equations in metals as a linear, isotropic, homogeneous, and non-magnetic medium.

$$\begin{aligned} \nabla \cdot \vec{D} &= 0, \\ \nabla \cdot \vec{B} &= 0, \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t}, \\ \nabla \times \vec{H} &= \vec{J} + \frac{\partial \vec{D}}{\partial t}. \end{aligned} \tag{1}$$

The electric displacement \vec{D} is given by:

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} \tag{2}$$

and \vec{P} is the polarization vector. For non-magnetic medium $\vec{B} = \mu_0 \vec{H}$, we can write the polarization $\vec{P} = \epsilon_0 \chi_e(\omega_0) \vec{E}$; hence, the electric displacement \vec{D} can be written as:

$$\vec{D} = \epsilon_0 (1 + \chi_e(\omega_0)) \vec{E} = \epsilon_1(\omega_0) \vec{E}, \tag{3}$$

where $\epsilon_1(\omega_0)$ is the real dielectric constant or the electric permittivity of the medium at given carrying frequency ω_0 . We conventionally assume that the linear relation between current \vec{J} and \vec{E} for isotropic medium as

$$\vec{J} = \sigma \vec{E} \quad (4)$$

here $\sigma(\omega_0)$ is the real constant that can be used to define the complex electric permittivity $\epsilon_r(\omega_0)$. The wave equation inside the lenses takes the form:

$$\nabla^2 \vec{E} - \epsilon_1 \mu_0 \frac{\partial^2 \vec{E}}{\partial t^2} = \sigma \mu_0 \frac{\partial \vec{E}}{\partial t}. \quad (5)$$

The index of refraction for X-rays inside the medium can be written as:

$$n = 1 - \delta + i\beta, \quad (6)$$

where δ for an appropriate materials is the refractive decrement of the order of $O(10^{-6})$ such that $1 - \delta$ close to one, while β is the absorption coefficient of the order of $O(10^{-9})$ [4, 5]. Thus, the material influences feebly the propagation of X-ray beams. Therefore, we can consider the field as a plane wave with the same wave number as in free space $k_0 = \frac{\omega_0}{c_0}$, the shift would be accounted for by the equation for amplitude A_{lens} inside the lens which is slowly dependent on \vec{r} and t . Hence

$$\vec{E}(\vec{r}, t) = A_{\text{lens}}(\vec{r}, t) \exp(i(k_0 x - \omega_0 t)) + c.c. \quad (7)$$

In conditions of a stationary source, we obtain:

$$\frac{\partial A_{\text{lens}}}{\partial x} + \frac{i\omega_0}{2c_0} \left(1 - \epsilon_1 \mu_0 c_0^2 - \frac{i\mu_0 \sigma c_0^2}{\omega_0} \right) A_{\text{lens}} = \frac{ic_0}{2\omega_0} \left(\frac{\partial^2 A_{\text{lens}}}{\partial y^2} + \frac{\partial^2 A_{\text{lens}}}{\partial z^2} \right), \quad (8)$$

the complex permittivity and the index of refraction n are linked by the relation

$$n = \sqrt{\epsilon_r \mu_0}, \quad (9)$$

where μ_0 is close to 1. Hence, we can express the index of refraction n as $n = \sqrt{\epsilon_r}$, and

$$\frac{\partial A_{\text{lens}}}{\partial x} + \frac{i\omega_0}{2c_0} (1 - n^2) A_{\text{lens}} = \frac{ic_0}{2\omega_0} \left(\frac{\partial^2 A_{\text{lens}}}{\partial y^2} + \frac{\partial^2 A_{\text{lens}}}{\partial z^2} \right). \quad (10)$$

But, while

$$n^2 = 1 - 2(\delta - i\beta) + (\delta - i\beta)^2 = \epsilon_r, \quad (11)$$

we can neglect the term $(\delta + i\beta)^2$ since it is very small compared to other terms. Now equation (10) takes the form:

$$\frac{\partial A_{\text{lens}}}{\partial x} + B A_{\text{lens}} = \frac{ic_0}{2\omega_0} \left(\frac{\partial^2 A_{\text{lens}}}{\partial y^2} + \frac{\partial^2 A_{\text{lens}}}{\partial z^2} \right), \quad (12)$$

where

$$B = \frac{\omega_0}{c_0} (i\delta + \beta). \quad (13)$$

For propagation in free space, it is a special case of equation (12) with $B = 0$, and $A_{\text{lens}} = A$ the complex amplitude in free space. Thus, in free space we have the parabolic equation:

$$\frac{\partial A}{\partial x} = \frac{ic_0}{2\omega_0} \left(\frac{\partial^2 A}{\partial y^2} + \frac{\partial^2 A}{\partial z^2} \right), \quad (14)$$

2.2. The geometry of the lens and boundary conditions

In this model we consider compound refractive lenses with the same shape as in [1] each of which has a parabolic cross section of width (lens) = 1 mm, and the smallest width of lens (d). We indicate the curvature radius at $y = z = 0$ of the lens as R [1]. Using the equation of parabola we can define the left and right surface of a lens as:

$$\begin{aligned} XSL(y,z) &= -0.5R((y - 0.5lenw)^2 + (z - 0.5lenw)^2) + \left(\frac{lenw - d}{2}\right), \\ XSR(y,z) &= 0.5R((y - 0.5lenw)^2 + (z - 0.5lenw)^2) + \left(\frac{lenw + d}{2}\right). \end{aligned} \tag{15}$$

At the boundaries, going from equation (14) to (12) we assume the amplitude function to be continuous, neglecting reflections due to a small deviation of the refraction index from 1. As initial condition (along x) we apply stationary case of coherent wave form (7).

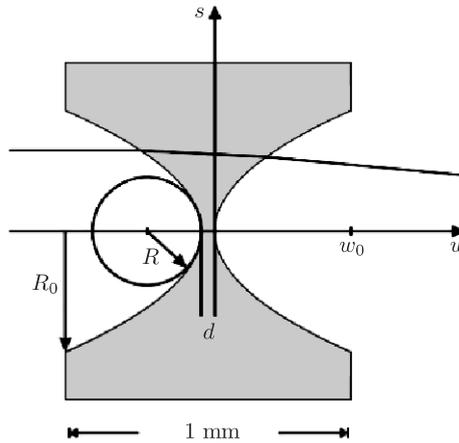


Figure 1. Single Parabolic lens. This figure is from [1]

3. The Numerical method

3.1. Implicit Runge-Kutta scheme

In this section we will solve equation (14) and equation (12) numerically using the finite-difference method, transforming the PDE (16) to the system of ODEs, and the implicit Runge-Kutta scheme of the second order with iterative procedure implementation [6]. We naturally account for continuity on a lens boundary.

Let us start with equation (12) for propagation inside the lens. We will denote that $A_{\text{lens}} = \tilde{A}$ just for simplicity

$$\frac{\partial \tilde{A}}{\partial x} + B\tilde{A} = \frac{ic_0}{2\omega_0} \left(\frac{\partial^2 \tilde{A}}{\partial y^2} + \frac{\partial^2 \tilde{A}}{\partial z^2} \right). \tag{17}$$

$$\frac{\tilde{A}_{j,k}^{n+1} - \tilde{A}_{j,k}^n}{h_{\text{lens}}} + B\tilde{A}_{j,k}^{n+\frac{1}{2}} = \frac{ic_0}{2\omega_0 h_r^2} \left(\tilde{A}_{j+1,k}^{n+\frac{1}{2}} + \tilde{A}_{j-1,k}^{n+\frac{1}{2}} + \tilde{A}_{j,k+1}^{n+\frac{1}{2}} + \tilde{A}_{j,k-1}^{n+\frac{1}{2}} - 4\tilde{A}_{j,k}^{n+\frac{1}{2}} \right), \quad (18)$$

where h_{lens} is the space step in x -axis inside the lens. In order to calculate intermediate quantities $\tilde{A}_{j,k}^{n+\frac{1}{2}}$ we apply the implicit scheme

$$\tilde{A}_{j,k}^{n+\frac{1}{2}} \left(1 + \frac{B \cdot \text{Dist}}{2} + \frac{ic_0 h_{\text{lens}}}{\omega_0 h_r^2} \right) = \tilde{A}_{j,k}^n + \frac{ic_0 h_{\text{lens}}}{4\omega_0 h_r^2} \left(\tilde{A}_{j+1,k}^{n+\frac{1}{2}} + \tilde{A}_{j-1,k}^{n+\frac{1}{2}} + \tilde{A}_{j,k+1}^{n+\frac{1}{2}} + \tilde{A}_{j,k-1}^{n+\frac{1}{2}} \right), \quad (19)$$

where Dist is the distance between two points inside the lens that needs to be defined according to the shape of our parabolic lens.

Finally we arrive at a simple formula

$$\tilde{A}_{j,k}^{n+1} = 2\tilde{A}_{j,k}^{n+\frac{1}{2}} - \tilde{A}_{j,k}^n. \quad (20)$$

The system of equations (19) and (20) gives us the implicit Runge-Kutta method of the second order [6].

For the propagation in free space, the scheme takes the form:

$$2\frac{A_{j,k}^{n+\frac{1}{2}} - A_{j,k}^n}{h_x} = \frac{ic_0}{2\omega_0 h_r^2} \left(A_{j+1,k}^{n+\frac{1}{2}} + A_{j-1,k}^{n+\frac{1}{2}} + A_{j,k+1}^{n+\frac{1}{2}} + A_{j,k-1}^{n+\frac{1}{2}} - 4A_{j,k}^{n+\frac{1}{2}} \right), \quad (21)$$

$$A_{j,k}^{n+1} = 2A_{j,k}^{n+\frac{1}{2}} - A_{j,k}^n. \quad (22)$$

3.2. Parameters of integration choice

Inside the lenses. From the dispersion relation for equation (12) the following conditions must be satisfied for the propagation inside the lenses

$$h_{\text{lens}} \ll \frac{w_0 h_r^2}{c_0}, \quad (23)$$

and

$$h_{\text{lens}} \ll \frac{1}{|B|}. \quad (24)$$

We take h_{lens} as the space step for x -axis inside the lens with the condition:

$$h_x \ll \frac{w_0 h_r^2}{c_0}. \quad (25)$$

The parameter h_x is the space step in x -axis in free space.

The first step

$$\tilde{A}_{j,k}^{n+\frac{1}{2}(0)} \left(1 + \frac{B \cdot \text{Dist}}{2} + \frac{ic_0 h_{\text{lens}}}{\omega_0 h_r^2} \right) = \tilde{A}_{j,k}^n + \frac{ic_0 h_{\text{lens}}}{4\omega_0 h_r^2} \left(\tilde{A}_{j+1,k}^n + \tilde{A}_{j-1,k}^n + \tilde{A}_{j,k+1}^n + \tilde{A}_{j,k-1}^n \right), \quad (26)$$

the second step, we need to run it for several times

$$\tilde{A}_{j,k}^{n+\frac{1}{2}(m+1)} = \frac{\tilde{A}_{j,k}^n + \frac{ic_0 h_{\text{lens}}}{4\omega_0 h_r^2} \left(\tilde{A}_{j+1,k}^{n(m)} + \tilde{A}_{j-1,k}^{n(m)} + \tilde{A}_{j,k+1}^{n(m)} + \tilde{A}_{j,k-1}^{n(m)} \right)}{\left(1 + \frac{B \cdot \text{Dist}}{2} + \frac{ic_0 h_{\text{lens}}}{\omega_0 h_r^2} \right)}, \quad (27)$$

the last step

$$\tilde{A}_{j,k}^{n+1} = 2\tilde{A}_{j,k}^{n+\frac{1}{2}(m)} - \tilde{A}_{j,k}^n. \quad (28)$$

Outside the lenses. If we put $B = 0$ in the equations, we will obtain the implicit scheme in vacuum outside the lenses. In calculations it is enough to take $m = 4$ [6].

4. Numerical simulations

In this part we will discuss our numerical results. We use the initial conditions at $x = 0$ as in [1] in order to compare the results. The initial conditions are Gaussian beams with $\text{FWHM} = 700 \mu\text{m}$ in the horizontal direction, and $\text{FWHM} = 35 \mu\text{m}$ in the vertical direction. We consider here two cases, the first case using the data from [1], and the second case with several lenses to perform the 2-d simulation. For the first case the results showed that we need to consider more than 50000 points in each direction, which will be difficult for the personal computer, therefore, we will only perform the 1-d simulation. While, for the second case we use a smaller number of lenses up to 15 lenses in order to perform the 2-d simulation.

4.1. First case 33 Al lenses with 15 keV X-ray

We consider the data from [1], and we test the program for a different number of points in each direction. The results should not depend on the number of points that we use in y, z directions (for y only in the 1-d case). In order to do that, we need to choose the h_x , and h_r space steps in x, y , and z directions, respectively, correctly and try to find a suitable number of points for our mesh. The dispersion relation governs the relation between the space steps in each direction $h_x \ll \frac{\omega_0 h_r^2}{c_0}$. In order to choose the number of points in y, z direction we need to calculate $0.001/h_r$, this relation will give us the number of points in the horizontal and vertical direction, h_x here is used as the space step in the x -axis to identify the place of the detector. For instance, if the focal plane is at 1.298 m from the CRLs it means that we need $1.298/h_x$ points in the x -axis. While, h_{lens} is used as the space step inside the lens, and it should satisfy the conditions in the dispersion relation for equation (12).

- Number of Al lenses = 33
- Radius of curvature = 0.2 mm
- Energy = 15 keV
- $\delta = 2.414 \times 10^{-6}$
- $\beta = 1.299 \times 10^{-8}$
- The distance from the source to the CRLs is 63 m

4.1.1. The choice of h_x

First, let us choose the best value for the constant in the relation

$$h_x = \text{constant} \times \frac{\omega_0}{c_0} h_r^2 \quad (29)$$

that will give us the best choice for the space step h_x . We fixed the number of points as 40000, which means that we fixed the space step h_r . We tried with some values for constant h_r , the results showed that the best choice for the space step was 0.032911422 which gave us a small error in the FWHM and in the focal distance, see Table 1. We can go further by choosing a smaller value for the constant which means a smaller value for h_x that will give us a smaller error. However, in this case we need more points for the propagation after the CRLs. For example, if we choose the constant to be 0.016455711 that gives us space step $h_x = 0.000000781$, and we need 1661440 points in the x -axis to reach the detector at 1.298 m.

Table 1. The choice of h_x

constant	h_x	focal distance	FWHM
0.131645688	0.00000625	1.2580312 m	3.25 μm
0.065822844	0.000003125	1.2539093 m	3.55 μm
0.032911422	0.000001562	1.2528818 m	3.65 μm

4.1.2. The error for choosing h_x

In order to compute the error we will use the Runge rule [7]. We can assume that $Z_h=3.55$ and $Z_{2h}=3.65$ for the spot size. The error can be written as

$$R = \frac{Z_h - Z_{2h}}{3} = 0.033333333 \quad (30)$$

which is small if we compare it to $\text{FWHM} = 3.65$. We can do the same for the focal distance f if $Z_h = 1.2539093$, $Z_{2h} = 1.2528818$, then

$$R = \frac{Z_h - Z_{2h}}{3} = 0.0003425 \quad (31)$$

which is very small if compared to 1.2528818. From the last investigations we can say that the best choice for the constant in the relation

$$h_x = \text{constant} \times \frac{\omega_0}{c_0} h_r^2 \quad (32)$$

is 0.032911422 which is equivalent to $h_x = 0.000001562$.

4.1.3. The choice of h_{lens}

Now, having obtained the best choice for $h_x = 0.000001562$ which is corresponding to constant 0.032911422 in the relation

$$h_x = \text{constant} \times \frac{\omega_0}{c_0} h_r^2 \quad (33)$$

We need to choose the space step inside the lens h_{lens} that will give us a small error according to the Runge rule for the spot size, and for the focal distance. We fix here the number of points to be 40000 which means that $h_r = 0.000000025$.

We have seen from the dispersion relation for the propagation inside the lens that the following conditions have to be satisfied

$$h_{\text{lens}} \ll \frac{w_0 h_r^2}{c_0} \quad (34)$$

and

$$h_{\text{lens}} \ll \frac{1}{|B|} \quad (35)$$

$\frac{1}{|B|} = 5.4533 \cdot 10^{-6}$. Table 2 gives us different values for h_{lens} with the corresponding spot size and focal distance. As can be seen the best choice for h_{lens} is 0.000000125 that will give us a small error according to the (Runge rule) for the spot size, and for the focal distance. The best choice for h_{lens} corresponding to 8000 steps for each lens.

Table 2. The choice of h_{lens}

h_{lens}	focal distance	FWHM
0.000001	1.2528818 m	3.65 μm
0.0000005	1.2492204 m	3.90 μm
0.00000025	1.2483004 m	3.95 μm
0.000000125	1.2480707 m	3.95 μm

4.1.4. Choice of h_r

In order to find necessary number of points for the mesh in the transverse plane, we need to find the suitable value for the space step h_r . We have fixed here the space step inside the lens $h_{\text{lens}} = 0.000000125$, we use the best choice for the constant to obtain h_x from the relation

$$h_x = \text{constant} \times \frac{\omega_0}{c_0} h_r^2 \quad (36)$$

which is equivalent to 0.000001562 for 40000 points, and 0.000001 for 50000 Table 3. Due to the large number of lenses, we need to consider more points, we started with 40000 points, and checked 50000 points. However, the results for 40000, and 50000 points are very close for the focal distance, and for the FWHM. We could take more points which means smaller h_r , and h_x . However, we use here the implicit Runge-Kutta method of the second order which means that we need to take 80000 points as the next step after 40000, not 50000. However, due to the limitations in the computer we will consider only 50000 points. We can say that, as a starting point, it is enough to consider 50000 points. In the future we will have to try with more points using supercomputers, and also for the 2-d case. In other words, the suitable choice of h_r will be 0.00000002.

Table 3. The choice of h_r

Number of points	h_r	focal distance	FWHM
40000	0.000000025	1.2480707 m	3.95 μm
50000	0.00000002	1.2470340 m	3.92 μm

5. Results for ideal lenses

We obtained the best choice for the space steps h_x , h_{lens} and h_r which correspond to using 50000 points. Our results give focal distance $f = 1.2470340$ m, and $\text{FWHM} = 3.92 \mu\text{m}$ at 1.298 m from the CRLs, Figure 2. We considered ideal lenses without any defects which was the main reason for having smaller FWHM than the experimental data. We considered only the 1-dim case for the horizontal direction while in the experimental data the horizontal and vertical results will be seen, Figure 3. Table 4 presents a comparison between our results and the experimental data. The results show that we have a good agreement with the experimental data for the focal distance, and for the intensity at the focal plane,

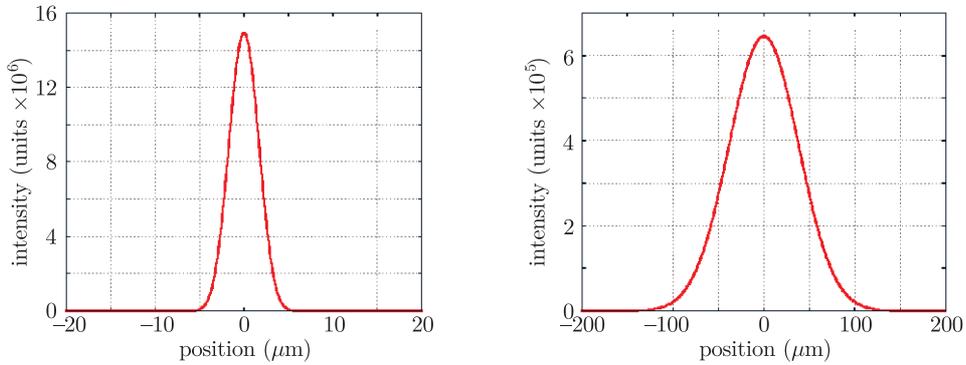


Figure 2. Results for Focusing hard X-rays with 33 perfect Al CRLs directly after the lenses (right), and at 1.298 m from the lenses (left) with $\text{FWHM} = 3.92 \mu\text{m}$, and focal distance = 1.2470340 m

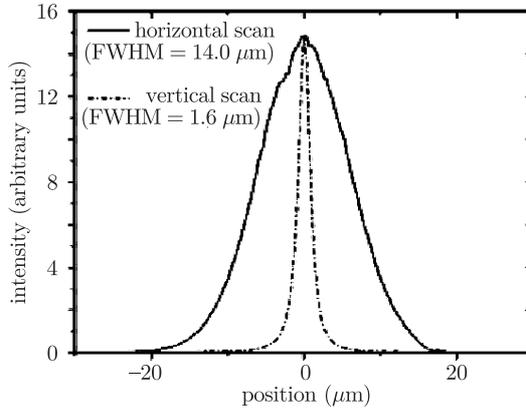


Figure 3. Experimental data for the horizontal and vertical direction [1]

Table 4. Comparing the Results

Item	focal distance	FWHM
Our results (Ideal CRLs)	1.2470340 m	$3.92 \mu\text{m}$
Experimental data	1.2553036 m	$14.0 \mu\text{m}$

while in case of the FWHM we have a smaller FWHM. We believe that is perhaps due to the ideal CRLs that we used and the fixed frequency.

6. Two-dimensional simulation

In this section we perform simulation for the 2-dimensional case. We obtain more than 50000 points in each direction from the last section that we need to consider in order to obtain accurate results, which makes it difficult to make a 2-d simulation for the first case using the PC. In this section, we only want to test the program for getting results in 2-d. We perform simulations here with fewer lenses up to 15 lenses made of Al. We use the same parameters as in the first case, but we consider the initial condition to be the same everywhere. Figure 4 and Figure 5 give us the results directly after the lenses. When we increase the number of lenses, the maximum value of the intensity decreases as absorption increases with the number of lenses.

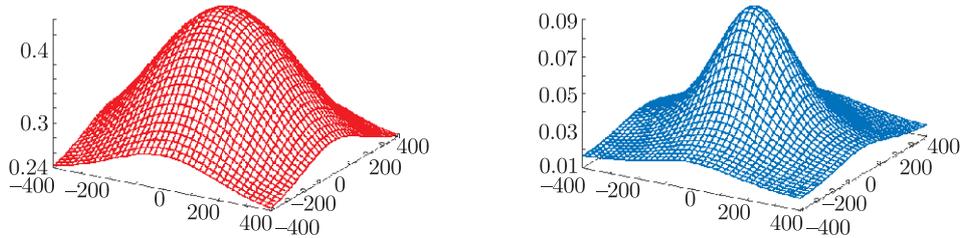


Figure 4. 2-Dimensional results for 1 lens (left) and 5 lenses (right)

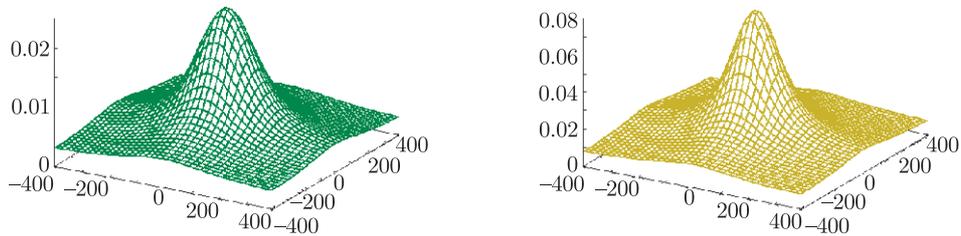


Figure 5. 2-Dimensional results for 10 (left) and 15 lenses (right)

7. Conclusion

We present here a new numerical method based on the finite-difference method to focus X-rays using CRLs. We solve the wave equation inside and outside lenses using the FDM and the implicit second order Runge Kutta method with the iterative procedure implementation. The program is written in FORTRAN to compute the focal distance and the spot size and cross structure. We considered here two cases with the same shape of the lenses as in [1]. As the first case we considered 33 Al lenses with a 15 keV beam having good agreement with the experimental data for the focal distance and for the intensity at the focal plane, while we have smaller results for the FWHM. We believe that the smaller

FWHM for the Gaussian beam appear because we use ideal lenses without any defects. The results showed that we needed to use more than 50000 points in each direction which forced us to perform one-dimensional simulation only. The time of calculation increased 16 times for the same number of lenses while the quantity of points in each direction increased two times which was due to the condition $h_x \ll \frac{\omega_0 h_r^2}{c_0}$. It means that if we compare a system of 100×100 points with a system of 1000×1000 for such a number of lenses we need to do 10000 times more operations than in the first case. The maximum quantity of complex points which could be calculated nowadays on a personal computer is about 5000×5000 to 10000×10000 . Hence, the program should be properly optimized and parallelized to perform the 2-d simulation using a supercomputer. In the second case, we tested the program for a small number of lenses up to 15 lenses made of Al. In the future, we will try to add some defects to the lenses, and check the influence of the defects on the spot size and on the focal distance. We also will take into account incoherence of the incoming beam to compare in details the results of calculation with experiments.

Acknowledgements

We would like to thank Prof. Sergey Kshevetskij and Dr. Pawel Wojda for their help in developing the numerical scheme. We are also grateful to Dr. Victor Kohn for consultations. The work is supported by the Ministry of Education and Science of the Russian Federation (Contracts Nos. 14.Y26.31.0002 and 02.G25.31.0086)

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