JOURNAL OF NANO- AND ELECTRONIC PHYSICS
Vol. **16** No 2, 02021(6pp) (2024)

ЖУРНАЛ НАНО- ТА ЕЛЕКТРОННОЇ ФІЗИКИ
Том **16** № 2, 02021(6cc) (2024)

REGULAR ARTICLE

Modeling of X-Ray Phase Contrast Imaging of Optically Heterogeneous Objects

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(Received 10 January 2024; revised manuscript received 18 April 2024; published online 29 April 2024)

The work relates to the study of the internal multi-layered structure of optically inhomogeneous objects by the X-ray phase contrast imaging method, which is an urgent issue of modern science, technology, nuclear physics and medicine. X-ray phase-contrast imaging makes it possible to examine weakly absorbing objects, reduce the radiation dose and increase the spatial resolution. Computer modeling of X-ray diffraction within the Fresnel-Kirchhoff scalar diffraction theory was used as the research method. An algorithm was developed for creating a model of a multilayer object with different values of the refraction decrement, which allows to specify the shape, size, number and thickness of layers, and the refractive index of each layer of the object. X-ray phase-contrast image was obtained for a multilayer object with a proportional decrease in the refraction decrement from the center to the edges by the free propagation approach. A comparative analysis was carried out with an X-ray image of a homogeneous object of the same size and shape. It is shown that the modeling result contains quantitative information about the internal structure of the object and its multi-layered nature.

Keywords: Multilayer object, X-ray Phase Contrast imaging, X-ray Diffraction, Fresnel-Kirchhoff Diffraction Theory, Phase Profile.

DOI: 10.21272/jnep.16(2).02021 PACS numbers: 42.25.Bs, 42.30.Va

1. INTRODUCTION

In practice, we often encounter objects with the internal heterogeneous or multilayer structure. For example, in living nature, such objects as the cornea, skin, blood, and other biological tissues have a complex multilayered structure with various mechanical, chemical, optical, electrical, and other properties [1-4]. There are also many similar objects in non-living nature. In particular, in metallurgy and materials science, a method of rapid cooling of liquid alloys is used, (hardening), as a result of which the outer layers of the material solidify quickly forming a fine-grained structure, while the inner layers do not have time to cool and the atoms form a coarser-grained structure. The multilayer structure is also often formed owing to industrial and technological surface treatment in a whole range of applications, in particular on structural elements of accelerator systems. We should also note the relevance of the study of multilayer objects for nuclear energy. Thus, nuclear fuel TRISO (TRi-structural ISOtropic particle fuel) for new generation reactors have a multi-layered structure, each layer of which has its own functions and physical properties [5]. Quality control of the production of these particles is mandatory. In addition, many materials, such as gradient optical materials, photonic crystals, and metamaterials, are specifically engineered with heterogeneous structures to achieve specific optical properties.

It is obvious that non-destructive research methods have significant advantages for both the study of materials and medical diagnostics. Many of these methods are based on the interaction of X-ray radiation with matter, since X-ray has a relatively high penetrating ability [6, 7]. Depending on the method and the area of research, sources with different values of X-ray parameters are used (intensity, wavelength, spectral and angular distribution, degree of coherence). Such facilities constantly needs improvement, minimization of geometric dimensions and harmful effects on living organisms, growing of resolution, cheapening and simplification of its production, etc. [8].

Among the numerous methods of research, X-ray phase contrast imaging (PCI) methods should be noted, which are based on the refraction phenomenon and processing of phase information after radiation-matter interaction. These methods have significant advantages, in particular, when studying weakly absorbing objects, reducing the radiation dose, increasing the spatial resolution. The implementation of PCI methods requires high values of X-ray parameters and sensitive high-resolution detector systems.

In recent years, a very powerful tool for the results of experimental research is computer modeling, which allows us to effectively simulate physical processes, calculate parameters that are difficult to obtain experimentally, improve our understanding of phenomena, and helps to check the correctness of theoretical models, etc. [9].

Thus, the aim of the presented work is the study of objects with a multilayer structure using PCI methods, which is an actual problem for modern science, technology, energy and medicine. We propose a new approach in computer modeling of the formation of a phase-contrast

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Cite this article as: A.Yu. Ovcharenko et al., *J. Nano- Electron. Phys.* 16 No 2, 02021 (2024) https://doi.org/10.21272/jnep.16(2).02021

X-ray image of three-dimensional objects with arbitrary geometric shape, which have a layered internal structure with different refractive indices of each layer. The presented study is intended for the further development of methods for modeling the interaction of X-ray radiation with matter. The results can be used for applied calculations of relevant experiments and determination of the potential capabilities of an experimental facility.

2. MODELING METHODOLOGY

2.1 X-ray Source Parameters and Optical Properties of the Object

X-ray phase contrast image is practically diffraction pattern. Modeling of PCI formation requires correct parameters to describe the properties of the object and the source to obtain accurate results. When X-ray radiation passes through an object, it is refracted and absorbed. This can be characterized on a macroscopic level using the complex index of refraction n:

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

where δ – refraction decrement; β – absorption coefficient. The value of δ depends on the chemical composition, the density of the material of the object, and the wavelength of the incident radiation. This parameter determines the phase shift and the amplitude of the secondary waves scattered by the object, which significantly affects the diffraction pattern. Ignoring the refraction decrement can lead to significant errors in calculations. In our study, we created three-dimensional computer models of the studied samples with a maximum size of the order of $l \sim 10^{-1}$ mm. X-ray radiation has a high penetrating ability through object, which can exceed object size by several orders of magnitude. Therefore, absorption of X-ray in the studied samples is not considered in our modeling, i.e., $\beta = 0$.

The phase shift of the X-ray wave that passed through the sample depends on the variations of the refraction decrement δ inside the sample and on its thickness. In the case of a monochromatic wave propagating along the z axis, the phase shift can be written in the following form [10]:

$$\varphi(x, y) = -\frac{2\pi}{\lambda}\int \delta(x, y, z)dz, \qquad (2)$$

where the integral is calculated over the thickness of the object in the direction of propagation of the X-ray beam. Note that the formula (2.2) can also be used to calculate to calculate the phase shift when X-rays pass through a multilayer object.

Real X-ray sources have always the emission spot of finite size and the certain spectral width. To obtain required degree of spatial coherency, typical dimensions of the source spot should be of the order of micrometers. The spectral width leads to the superposition of diffraction patterns with their weighted contribution for different wavelengths, which corresponds to the spectral distribution of radiation. Therefore, important parameters in calculating the intensity and profile of diffraction maxima and minima are the refraction decrement of the object δ and the degree of spatial and temporal coherency. Taking these parameters into account makes it possible to build accurate and realistic diffraction models.

Taking into account the degree of spatial coherency of the sources in image formation, is not aim of this study. To simulate X-ray diffraction on various objects, a monochromatic point source with a wavelength of $\lambda = 1.5 \cdot 10^{-4}$ μm was chosen.

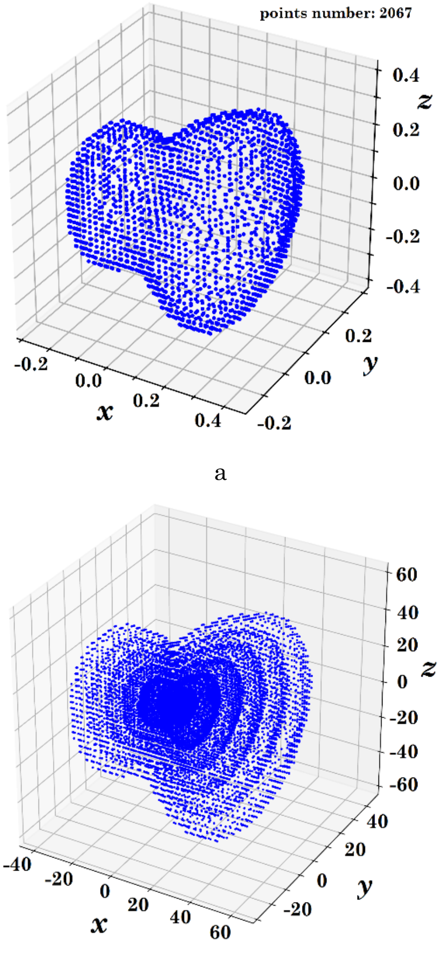
2.2 Creating Objects of Research

X-ray diffraction on a multilayer object with a non-uniform distribution of the refractive index was modeled in this paper. The object consisted of 6 layers (shells). To create such an object, the following steps were performed.

1) We select some arbitrary irregular geometric shape of the object using an analytical formula

$$36x^2 + 100y^2 + 56.25z^2 - 3\cos(1.5x) + \\ + \sin(1.5y) \le 4.3\sin(3x) \qquad (3)$$

and obtain the geometric location of the points that form the surface of this sample (see Fig. 1a). In this figure, all points lie inside a cube with a side of 1 μm. Note that the analytical criterion (3) was chosen arbitrarily, and its type and geometric parameters are not important for the calculation scheme.



a

b

Fig. 1 – Creation of a computer model of the research object: (a) geometric location of points for the formation of layers (shells); (b) the studied sample, which consists of 6 layers

2) We calculate the coordinates of the points that form the surfaces of the 6 layers of the object under study, using the method of similarity of shapes (Fig. 1b). Values along axes and cell size for the points that form the object are specified in μm.

The coordinates of all points shown in figure 1a were multiplied by the values 25, 50, 75, 100, 125 and 150 to obtain all points of the studied sample (Fig. 1b). Such a simple approach allowed us to create a model of multilayered object. The area of the object is a cube with a side of 150 μm. This method can be successfully applied for any number of layer and in the case when different layers of the object are not similar shapes.

3) To complete the creation of the sample model, each layer was assigned a refraction decrement value $\delta_1, \delta_2 \ldots \delta_6$ starting from the center of the object

$$10^{-6},\ 9 \cdot 10^{-7},\ 8 \cdot 10^{-7},\ 7 \cdot 10^{-7},\ 6 \cdot 10^{-7},\ 5 \cdot 10^{-7}. \quad (4)$$

The decrement values in Eq. (4) are characteristic for light materials, in particular, biological objects

Therefore, a very flexible and versatile method of creating a multilayer object was developed. It allows generating models of the studied samples with any shape, size, number of layers, and with any functional distribution of the refraction decrement across layers.

2.3 Analytical Model

The calculation of the PCI image of the multilayer object (Figure 2b) was performed for PCI free propagation method using the Fresnel-Kirchhoff diffraction theory [10-12]. Figure 2a shows the general scheme of X-ray diffraction simulation used in work on an object of arbitrary geometric shape from a point source of unit amplitude. Vectors $\boldsymbol{s}_i$ and $\boldsymbol{r}_i$ was specified for each X-ray propagation direction The thicknesses d_i of the sample and the corresponding phase shifts were calculated. The same calculations were performed for each layer of an object.

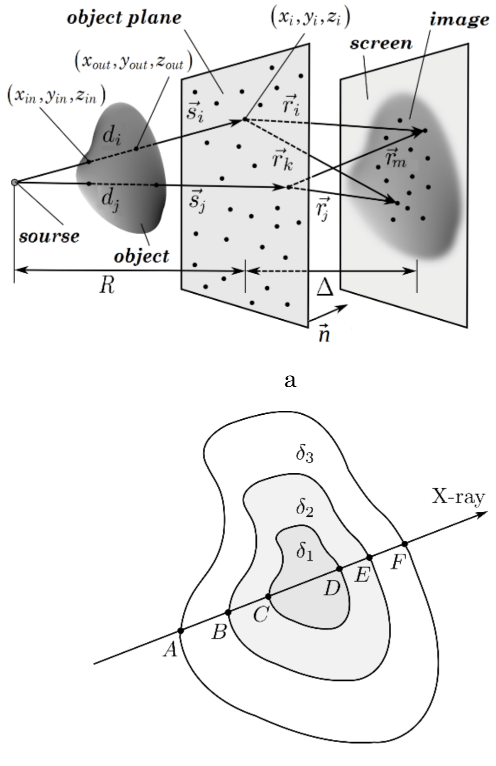
According to the Fresnel-Kirchhoff theory the complex scalar amplitude of X-ray described field on the screen plane can been write in the form [10-12]:

$$\psi(x_{scr}, y_{scr}) = \frac{1}{i\lambda} \iint_{-\infty}^{\infty} \frac{exp\big(ik(r+s)\big)}{rs} \times \frac{cos(\boldsymbol{n},\boldsymbol{r}_i)+cos(\boldsymbol{n},\boldsymbol{s}_i)}{2} \cdot exp(i\varphi) \cdot dx_i dy_i\ , \quad (5)$$

$$s = \sqrt{(x_i - x_s)^2 + (y_i - y_s)^2 + R^2}, \quad (6)$$

$$r = \sqrt{(x_i - x_{scr})^2 + (y_i - y_{scr})^2 + \Delta^2}. \quad (7)$$

Here λ – wavelength; $k = 2\pi/\lambda$ – the wave number; $\boldsymbol{s}_i$ – the vector directed from the source to a certain point on the object plane, $\boldsymbol{r}_i$ – the vector from the point on the object plane to the screen observation point; $\boldsymbol{n}$ – normal vector to the object plane; R – source-object distance; Δ – object-screen distance; φ – an additional phase shift that occurs after radiation passes through an object due to its optical properties. In the Eq. (5), integration is carried out over the object plane. The variables x_s and y_s are transverse coordinates of the source, the longitudinal coordinate is determined by the value R. The square of the module of complex amplitude (5) specified intensity distribution on the screen that is the form of diffraction pattern.



a

b

Fig. 2 – X-ray diffraction simulation scheme (a). Calculation of phase shifts when X-rays pass through the object (b): $d_1 = CD$, $d_2 = BE$, $d_3 = AF$

Let's consider the method of calculating the phase shifts of X-rays, when the research object has a heterogeneous structure. Figure 2b schematically shows, for example, a multilayer object consisting of three components with refraction decrements δ_1 , δ_2, δ_3 and corresponding thicknesses $d_1 = CD$, $d_2 = BE$, $d_3 = AF$. Then, according to the formula (2), the phase shift φ caused by the object will be equal to:

$$\begin{aligned} \varphi &= -\frac{2\pi}{\lambda}\big[\delta_1 CD\ + \delta_2(BC + DE) + \delta_3(AB + EF)\big] = \\ &= \ -\frac{2\pi}{\lambda}\big[\delta_1 \cdot d_1\ + \delta_2 \cdot (d_2 - d_1) + \delta_3 \cdot (d_3 - d_2)\big]. \quad (8) \end{aligned}$$

The above-described method of calculating phase shifts is universal and does not depend on the geometric shape, number, and dimensions of the shells of a multilayer object.

It is obvious that the greater the thickness of the studied sample and the greater the refraction decrement, the greater will be the X-ray phase shift. Figure 3 shows phase displacement maps in the object plane for a multilayer sample with refraction decrements of layers in according to Eq. (4) and for optically homogeneous samples that have exactly the same geometric dimensions as multilayer sample, but the refraction decrements are constant values $5 \cdot 10^{-7}$ (Fig. 3a), $7.5 \cdot 10^{-7}$ (Fig. 3b) and 10^{-6} (Fig. 3c).

The average value of the refraction decrement for a multilayer sample is equal to $7.5 \cdot 10^{-7}$ (Fig. 3d). If compared with an optically homogeneous sample, with a constant refraction decrement $7.5 \cdot 10^{-7}$ (Fig. 3b), we have small differences in the degree of phase shift change near the center of the studied samples.

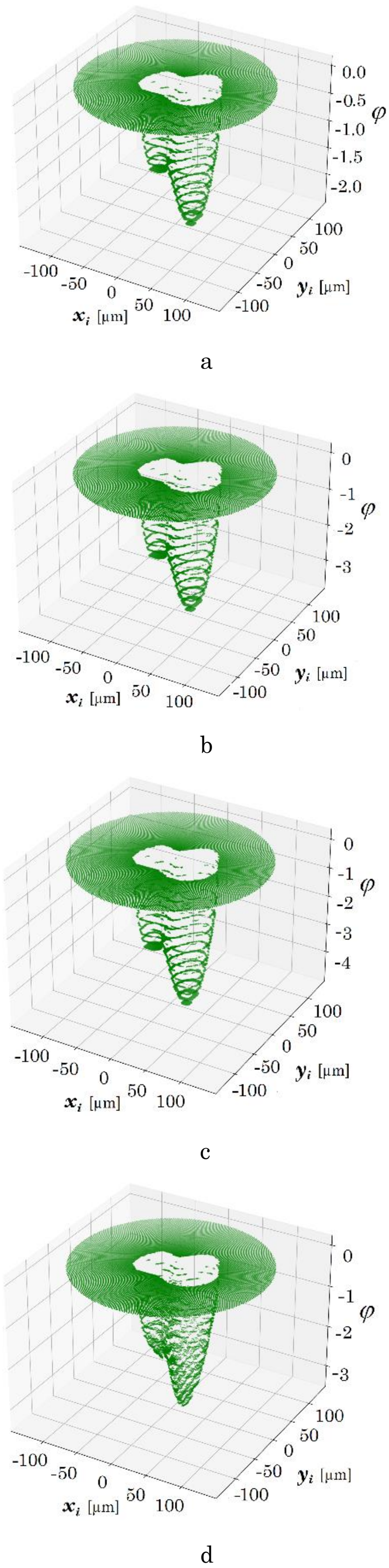


Fig. 3 – X-ray phase shift maps in the plane of the object: a, b, c – optically homogeneous samples with refraction decrements $\delta = 5 \cdot 10^{-7}$, $\delta = 7.5 \cdot 10^{-7}$ and $\delta = 10^{-6}$, respectively; d – a six-layer sample with the values of refraction decrements of layers in according to Eq. (4)

For optically homogeneous samples that have smaller (Fig. 3a) and larger (Fig. 3c) refraction decrements compared to the average value of the refraction decrement of a multilayer sample, we have, accordingly, different values of the maximum phase shifts of X-rays. This fully corresponds to the formula (5). The results of calculations of phase shifts caused by the passage of X-rays through the studied objects allow us to conclude that our proposed modeling method is sufficiently sensitive to changes in the optical properties of materials and may be suitable for modeling the diffraction of X-rays on optically inhomogeneous samples.

2.4 Numerical Parameters of Simulation

As mentioned above, the formulas (5)-(8) makes it possible to calculate the complex amplitudes of the diffraction pattern in the plane of the screen (detector) from a point source. In the general case, the integration should be carried out for an infinite plane of the object, which is impossible. Therefore, the calculation was carried out on the basis of numerical methods, by cutting the plane of the object. The plane of the object was selected as a circle with a radius of 130 μm and divided into 751 points along the azimuthal angle and 375 points along the radius (281625 points). The screen area with a radius of 300 μm was placed at a distance of 1.5 m from the object plane and divided into 301 points along the azimuthal angle and 150 points along the radius (45.000 points). According to these parameters, Figure 4 shows the intensity distribution obtained in the absence of the object, which does not have significant fluctuations in the center and shape of the diffraction pattern (Fig. 4b) from the edges corresponds to the well-known result [10].

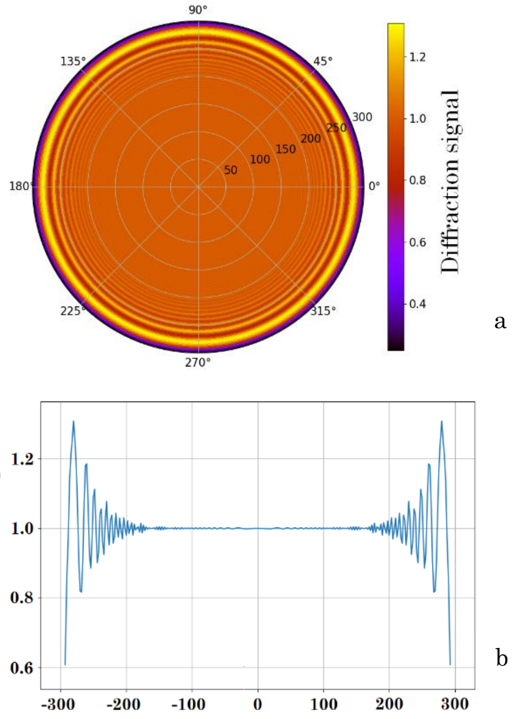


Fig. 4 – Diffraction image in the absence an object (a) and the corresponding intensity profile along the x -axis (b)

It indicates the correct choice of modeling parameters and allows to perform further computer simulation for PCI image of created object (see Fig. 1b).

3. RESULTS AND DISCUSSION

In this work, a computer simulation of PCI image of was performed for optically heterogeneous object shown in Figure 1b, which consists of 6 layers (shells) with different refraction decrements. In order to exclude the influence of the edges of the aperture on the image of the diffraction pattern in the area of the screen, we subtracted the distribution of intensity in the absence of the object from the intensity distribution of X-rays, which was obtained in modeling in the presence of an object the distribution of intensity in the absence of an object (Fig. 4). As a result, we receive pure images of the samples on the screen (see Fig. 5).

Note that this method is often implemented in practice of an experiment. Indeed, having the signal of intensity in the absence of research object and in the presence of an object, it is possible to obtain intensity distribution caused just the properties of object.

Fig. 5a shows the PCI image of multilayer object with the values refraction decrements in according to Eq. (4). To determine the sensitivity of our calculation model to changes in optical properties, we also calculated the diffraction of X-rays from an object that has exactly the same geometric shape and dimensions as a multilayer sample, but with a constant decrement of refraction $\delta = 7.5 \cdot 10^{-7}$ (Fig. 5a). This value of the refraction decrement for a homogeneous sample was chosen equal to the average value for a multilayer object, which is convenient for comparing the results.

The main differences in the intensity distribution for the objects studied in this work (see Fig. 5) are as follows. In the case of a homogeneous object, all secondary waves scattered by its various neighboring points have practically the same phase shift. At the same time, the phase shift changes smoothly with the sample thickness. For a multilayer object, these phase shifts are significantly different at the boundary of the layers due to the inhomogeneity of the refraction decrement. This leads to a change in the interference pattern. This is especially visible in the area where the samples have the smallest thickness throughout the cross-section (these are the radial directions with azimuthal angles 90^0 and 270^0, shown in Fig. 5 (a), (b)). There are also other minor differences in the intensity distribution, which can be found when comparing the images visually and when analyzing the intensity profiles (see Fig. 5 (c), (d)).

In this work, we aimed to develop a method of modeling X-ray diffraction on objects that have a layered structure and, as a result, exhibit anisotropic optical properties. The developed method should be sensitive even for slightly changes of the refractive indices inside the object. It explains the choice of refraction decrement value from $\delta = 5 \cdot 10^{-7}$ to $\delta = 10^{-6}$. Sensitive of method is important because the optical heterogeneity of objects can causes blurring of diffraction maxima and can also lead to the additional diffraction maxima. All this complicates the interpretation of the data.

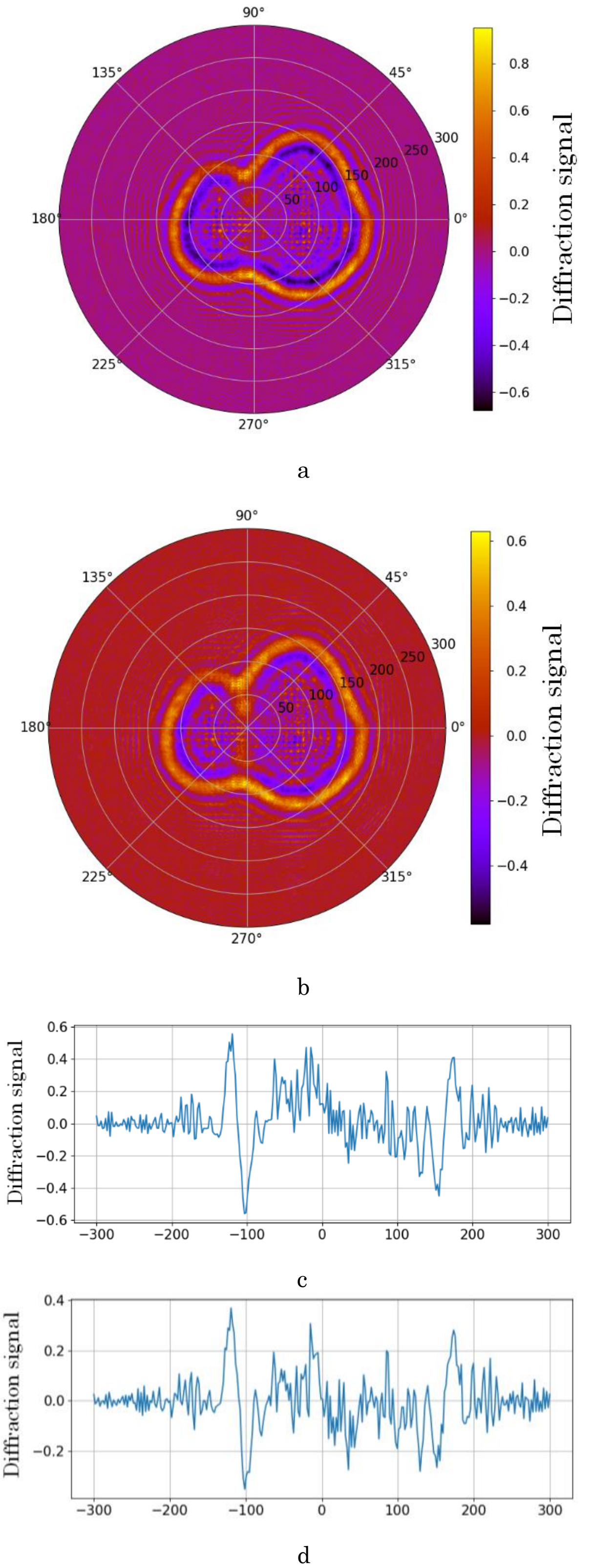


Fig. 5 – Pure diffraction images of the studied objects and intensity profiles along the the x -axis: (a),(c) – optically homogeneous sample with a refraction decrement of $7.5 \cdot 10^{-7}$; (b), (d) – a six-layer object with refraction decrements of layers in according to Eq. (4)

Note that the modeling result on Fig. 5b contains quantitative information about the internal structure of the object and indicates its multi-layered nature. Thus, we can claim that the approach developed for modeling X-ray diffraction on optically heterogeneous objects is suitable for practical use. It can be useful for developers of medical, scientific, industrial and other equipment, the basis of which is the phenomenon of X-ray diffraction.

4. CONCLUSIONS

The study of the optically inhomogeneous objects is urgent issue of modern science, technology, nuclear physics and medicine. In this work, a modeling technique of the X-ray phase contrast image of multilayer objects was developed within the Fresnel-Kirchhoff scalar diffraction theory. An algorithm was developed for creating a model of a multilayer object with different values of the refraction decrement, which allows to specify the shape, size, number and thickness of layers, and the refractive index of each layer of the object.

The results of calculations of phase shifts caused by the passage of X-rays through the studied objects was obtained over the object plane. Analysis shows that proposed modeling method is sufficiently sensitive to changes in the optical properties of materials and may be suitable for modeling the diffraction of X-rays on optically inhomogeneous samples.

X-ray phase-contrast image was obtained for a multilayer object with a proportional decrease in the refraction decrement from the center to the edges by the free propagation approach. The obtained diffraction results were compared with the case of a homogeneous object of the same size and shape.

It is shown that the modeling result contains quantitative information about the internal structure of the object and its multi-layered nature. It can be useful for developers of medical, scientific, industrial and other equipment, the basis of which is the phenomenon of X-ray diffraction.

ACKNOWLEDGMENTS

The work was supported by the state research project № 0122U000417 and the Grant of the NAS of Ukraine 2024-2025 of research groups of young scientists № 0124U002466.

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Моделювання рентгенівського фазоконтрастного зображення оптично неоднорідних об'єктів

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Робота стосується дослідження внутрішньої багатошарової структури оптично неоднорідних об'єктів методом рентгенівського фазового контрасту, що є актуальним питанням сучасної науки, технології, ядерної фізики та медицини. Рентгенівська фазоконтрастна візуалізація дозволяє досліджувати слабко поглинаючі об'єкти, зменшити дозу опромінення та підвищити просторову роздільну здатність. Методом дослідження було використано комп'ютерне моделювання дифракції рентгенівського випромінювання в рамках скалярної теорії дифракції Френеля-Кіргхофа. Розроблено алгоритм створення моделі багатошарового об'єкта з різними значеннями декременту заломлення, який дозволяє визначати форму, розмір, кількість і товщину шарів, показник заломлення кожного шару об'єкта. Отримано рентгенівське фазоконтрастне зображення в методі вільного поширення для багатошарового об'єкта із пропорційним зменшенням декременту заломлення від центу до країв. Проведено порівняльний аналіз із рентгенівським зображенням однорідного об'єкта такого ж розміру та форми. Показано, що результат моделювання містить кількісну інформацію про внутрішню будову об’єкта та його багатошарову природу.

Ключові слова: Багатошаровий об’єкт, Рентгенівське фазо-контрасне зображення, Рентгенівська дифракція, Теорія дифракції Френеля-Кірхгофа, Фазовий профіль.