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# Computer Simulation of the Zernike Phase Contrast in Hard X-Ray Radiation Using Refractive Lenses and Zone Plates

**V. G. Kohn[a] and M. A. Orlov[b]**

[a] *Russian Research Centre Kurchatov Institute, Moscow, Russia*

[b] *Lomonosov Moscow State University, Moscow, Russia*

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**Abstract**—Computer simulation of an experiment on imaging transparent (phase) microobjects using the Zernike phase contrast method under hard X-ray radiation has been performed. The beam parameters typical for synchrotron radiation sources of the third generation were used in calculations. Both a refracting lens and a zone plate have been considered as a focusing element. The phase shifting quarter-wave plate is located at a spot of the point source image. The results of calculations have shown that the method can be successfully used for objects with the sizes greater than 0.1 μm along and 1 μm across the beam. It has been shown that the contrast is caused not only by increasing the intensity within the shadow of the objects, but also by decreasing the intensity in the area beyond the objects, which is necessary to retain the integral intensity.

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## 1. INTRODUCTION

Hard X-ray radiation beams obtained by synchrotron radiation sources of the third generation have a high degree of spatial coherency. This allows one to observe coherent effects related to the change in the wave phase, of which the phase contrast method [1] has become most popular for the investigation of the internal structure of weakly absorbing noncrystalline objects. Its main advantage, as compared to the absorption contrast method, is that the change in the intensity due to the change in the phase incursion introduced into the wave front of incident beam by different object areas is investigated. Since the phase incursion is much faster than the change in the wave amplitude due to absorption, the phase contrast allows one to decrease substantially the absorbed radiation dose which can be important, for example, in the investigation of biological objects. However, in this method the phase changes transform into the change in the intensity at a certain distance from the object and, generally speaking, depend on this distance. The change at small distances is very weak and can be considered as local beam microfocusing or defocusing. The contrast increases at large distances, but the change in the intensity is similar to the hologram that should be reconstructed in order to obtain the structure of phase changes in the object.

Medical-biological samples with millimeter sizes are typical investigation objects in the phase contrast method. Along with this, this method in its initial form proves to be ineffective in going to micro- and nanoscales when the phase shift introduced by objects becomes rather small. The idea of using the Zernike phase contrast method [2] known from visible light optics in the X-ray wavelength range is quite attractive as an alternative approach. In optical investigations this technique is widely used for imaging transparent objects, whereas in the X-ray range it is currently insufficiently known. The method was used only in several experimental works [3–5] which were crowned with definite success. However, theoretical investigations have not been carried out. In the present work the computer simulation of the Zernike phase contrast method in the hard X-ray radiation range with the use of model objects and some modification of this method has been carried out. It has been shown that the method gains new properties in this frequency range, an account of which can further increase its efficiency.

## 2. ZERNIKE METHOD SCHEME FOR X-RAYS

The main difference in realization of the Zernike method in the optical and X-ray wavelength ranges is the following. As is known, a refracting lens is a key element in an optical scheme of phase contrast. In the X-ray range, the possibilities of refracting lenses began to be investigated only in 1996 [6], and methods have been developed, lenses have been prepared, and their properties as focusing and imaging elements have been tested [7]. The presence of a series of problems is a reason of this state. First of all, since X-rays have rather insignificant refraction factor, these lenses must have a very small radius of curvature and, consequently, a large length; therefore, the process of their preparation is rather labor-intensive.

In addition, there are no transparent materials for X-rays and focusing lenses are concave rather than convex. Therefore, they transmit radiation in the area

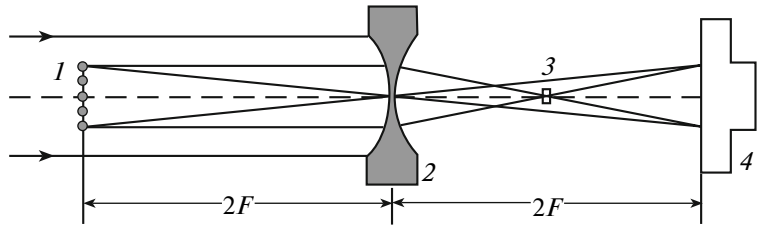


**Fig. 1.** Scheme of the Zernike phase contrast when a refracting lens is used. Almost parallel beam falls on the left side: (*1*) object, (*2*) refracting lens, (*3*) phase-shifting plate, (*4*) position detector. For the image without magnification, an object and detector are arranged at the double focal distance from the lens and a phase shifting plate is placed at the point of source focusing.

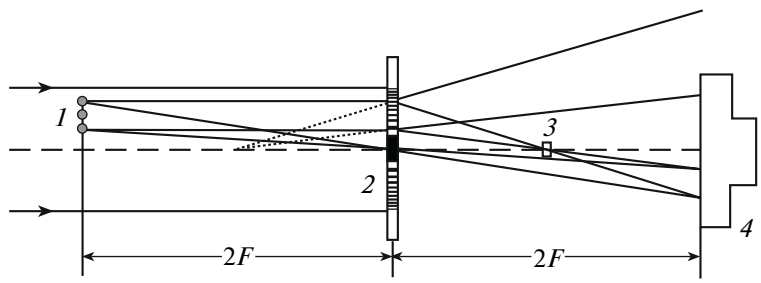


**Fig. 2.** Scheme of the Zernike phase contrast when a zone plate is used. Numbers denote the identical objects as in Fig. 1, but *2* is the zone plate. In the given case, the object is shifted from the optical axis to separate the effect of the first and minus first orders of focusing.

where material quantity is insufficient, but their aperture is determined by absorption rather than geometrical sizes, since X-ray travel a long path inside material when a beam trajectory is deviated from a lens center. For this reason, refracting lenses are used exclusively in the hard X-ray range when a role of absorption decreases as compared to a phase incursion. The formation of a two-lens system in the X-ray range and, especially, multilens systems for image formation is still beyond possibility. At the same time, it is known that the standard optical Zernike scheme includes three lenses, a collector collecting the radiation diverging from a source into an almost parallel beam, a condenser compressing a beam and directing it to a sample, and an objective.

At first glance it may appear that the use of the Zernike method for the X-ray range is an awkward problem. However, the possibilities of synchrotron sources of the third generation allow us to limit ourselves only to a single lens, the objective. Really, since a radiation source has rather small sizes of the order of 50 μm, and is moved away from the source to a large distance for about 50 m, the initial beam proves to be virtually parallel; therefore, there is no necessity for a collector. In addition, a condenser focusing a beam at an object to amplify illumination intensity becomes unnecessary, since synchrotron radiation has very high brightness. Thus, there are no principal limitations in the use of the Zernike method in the X-ray range. Nevertheless, to date lenses have not been used in practice as objectives, zone plates being used instead in all experimental works using the Zernike method, since the technique for preparation of zone plates is more developed. However, zone plates are not an ideal focusing element, which leads to image quality loss. In the given work, both cases have been considered, both a refracting lens and a zone plate as an objective. The experimental schemes considered for realization of the Zernike method are presented in Figs. 1 and 2.

## 3. CALCULATION METHOD

To solve the problem of hard X-ray radiation transfer and scattering, a paraxial approximation is carried out with a high accuracy. In this case radiation transfer in air is described by the integral Kirchhoff formula as the solution of the Maxwell equation. Let the $z$ axis in the Cartesian coordinate system be directed along the optical axis, namely, along the radiation beam propagation. The problem is to calculate the dependence of the wave field amplitude on the $x$ and $y$ coordinates at each point at the $z$ axis. In this case the characteristic range of the substantial change in the wave field along the $z$ axis is tens of centimeters, whereas the wave field changes in transverse directions at distances of several micrometers or less. Since polarization in the considered processes does not change, it is sufficient to limit ourselves to the scalar wave function of field. Moreover, to simplify the problem, we will consider only one-dimensional objects, being uniform along the $y$ axis.

Let $E_1(x)$ be the wave function at the $z_1$ point. Then under the condition that there are no objects between

$z_1$ and $z$, the wave function $E(x)$ at the $z$ point is determined by the following:

$$E(x) = \int dx_1 P(x - x_1, z - z_1) E_1(x_1),$$
$$P(x,z) = \frac{1}{(i\lambda z)^{1/2}} \exp\left(i\pi \frac{x^2}{\lambda z}\right). \quad (1)$$

Here $P(x, z)$ is the Kirchhoff propagator in the paraxial approximation and $\lambda$ is the radiation wavelength. As for the objects, it is possible to neglect the change in the beam trajectory when passing the object if their longitudinal sizes do not differ too much from transverse ones, since the scattering angles are quite small (usually tens of microradians). The length of the object along the optical axis can also be neglected, and the object can be considered as a plane one. Then the interaction of radiation with a uniform object is described by multiplying the wave function of radiation field by the so-called transmission function

$$T(x) = \exp\left(-i[\delta - i\beta]\frac{2\pi}{\lambda} t(x)\right), \quad (2)$$

where $t(x)$ is the local change in the object thickness along the $z$ axis under the condition that it consists of single material and $\delta$ and $\beta$ are the parts of the complex refractive index $n = 1 - \delta + i\beta$ of the material which the object consists of.

Calculation begins from a point source. The wave function at the point of source can be formally taken in the form of delta function $E_0(x) = \delta(x)$. Substituting this into (1) we immediately obtain the wave function in front of the investigated object in the form of the Kirchhoff propagator $E_1(x) = P(x, r_1)$, where $r_1$ is the distance from source to object. Then it is necessary to multiply the wave function by the transmission function of the object in which the dependence $t(x)$ must be concretely taken into account and Eq. (1) must be once more used. However the limits of integration in (1) are infinite, whereas the range of integration in the concrete numerical calculations is finite. Therefore we will assume in the calculations that the transmission function does not change beyond the limits of the concrete integration range and is constant, i.e., $T(x) = T_0$, where $T_0$ is described by Eq. (2) for $t(x) = t_0$. In particular, it is possible that $t_0 = 0$. Then the integral in (1) can be transformed into the form

$$E_2(x) = T_0 P(x, r_2)$$
$$+ \int dx_1 P(x - x_1, r_2 - r_1)[T(x)E_1(x_1) - T_0 P(x_1, r_1)]. \quad (3)$$

In this equation $r_2$ is the distance from the observation point to the source. In the general case, we assume that $E_1(x) = P(x, r_1)$ beyond the limits of the integration range. For the first calculation, this equality is fulfilled inside the integration range, but the situation is more complex for further calculations.

For the first calculation, $r_2$ is the distance from source to focusing lens (refracting lens or zone plate, Figs. 1 and 2). Then the calculation by Eq. (3) should be repeated with a new object in the form of a focusing lens. In this case the substitution $r_2 \to r_3$ and $r_1 \to r_2$ should be made, where $r_3$ is the distance from the source to the point of its focusing in which a phase shifting element is placed. In the case of the biconcave refracting parabolic lens, $t(x) = x^2/R$, where $R$ is the radius of curvature at the peak of parabola. In the given case, the infinite integration limits are effectively cut due to absorption in lens if a lens is sufficiently thick at the aperture edges. In the case of a zone plate, the absorption can be neglected and the problem with integration limits remains. A zone plate has a finite aperture, is uniform beyond aperture, and has the $t_0$ thickness. Inside the aperture a zone plate has $t(x) = 0$ in the zones where there is no material and $t(x) = t_0$ in the zones with material. The zone boundaries are described by the formula $x_n = r_1(n)^{1/2}$, where $r_1$ is the radius of the first zone and $n$ is the zone number. For the third calculation the phase shifting element with the sizes of order of the beam size in the lens focus is the object. In this case the substitution $r_2 \to r_4$ and $r_1 \to r_3$ should be made in Eq. (3), where $r_4$ is the distance from source to position detector.

The integral in (3) is a convolution of two complex functions, and its direct calculation is a rather complex problem. Therefore, the calculation was carried out using the Fourier transform. First of all, the Fourier transform of the function in square brackets is calculated; then it is multiplied by the Fourier transform of the Kirchhoff propagator, which has the analytical form $P(q, r) = \exp(-i\lambda r q^2/4\pi)$, and the inverse Fourier transform is calculated using the known procedure of the fast Fourier transform [8]. The computer program was written using the Java programming language [9].

## 4. THE CALCULATION RESULTS FOR THE SCHEME WITH LENS

The numerical experiment was carried out in accordance with the scheme presented in Fig. 1. A hard X-ray radiation source with the $S_0$ size was moved away from observation object *1* at the $r_1$ distance. Object *1* is placed at the double focal distance from X-ray refracting lens *2*, i.e., $r_2 - r_1 = 2F$. Phase shifting plate *3* is placed at the point of source image $r_3 = r_2 + F/(1 - F/r_2)$ determined by the lens formula. Detector *4* is placed at the distance $r_4 - r_2 = 2F$ from lens; therefore, the image is inverse and not increased.

For calculations the standard parameters of synchrotron sources of the third generation were chosen, namely, the distance from source to object $r_1 = 50$ m and the source size $S_0 = 50$ μm. A beryllium lens was considered as an object with the following parameters: the focal distance $F = R/2\delta = 20$ cm, the lens length $p = A^2/4R = 4.6$ cm, the radius of lens curvature $R = 0.88$ μm, and the geometric aperture $A = 400$ μm. The calculations were carried out for the energy of incident radiation $E = 12.4$ keV, which corresponds to the wavelength $\lambda = 0.1$ nm. The source is incoherent; this means that each of its points lights independently in phase. Since a source has a finite size $S_0$, its image in a focus will also have the definite size $S = S_0(r_3 - r_2)/(r_1 + r_2)$, and in our

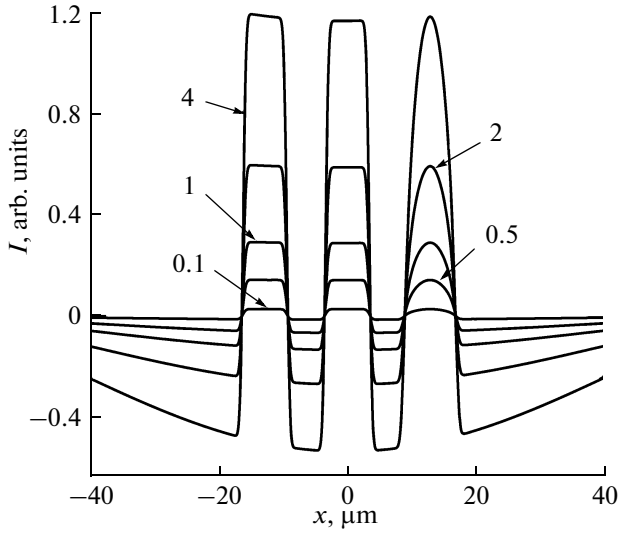


**Fig. 3.** Distribution of the difference in radiation intensities with and without objects in the Zernike method with a refracting lens for three objects with rectangular and circular cross section for the different values of longitudinal size *d*. The *d* values in μm are written at curves.

case this size is 0.2 μm, which exceeds the beam size under focusing of a point source (diffraction limit).

The source sizes were taken into account by calculation of the convolution of the intensity distribution of a point source with the Gaussian curve the half-width of which is $S_d = S_0(r_4 - r_2)/(r_1 + r_2)$. The radius of phase shifting plate was selected taking into account *S*. It should be noted that an absorbing lens results in the Gaussian distribution of intensity even in the absence of absorption objects, i.e., the intensity decreases at the aperture edges. To separate the object image in the pure state, a special method is frequently used in experiments; namely, the image is written in the object's absence and with the object, and then the first image is subtracted from the second one. The same method was used for the construction of graphs of the intensity distribution, i.e., to obtain the object image from the full intensity profile, the intensity profile formed by lens in the absence of object was subtracted.

We formulate the main problems of the numerical experiment with a refracting lens. First of all, it is necessary to analyze the applicability of the method, i.e., to recommend the object shape and size that can be principally observed by it. For this purpose the different small objects were considered, the sizes of which decreased down to the limit when these objects became already indistinguishable against a background. The image of three objects with rectangular and elliptic cross sections is shown in Fig. 3 for the different values of longitudinal size *d*. The minimal longitudinal size of the objects that can be still observed was about 0.1 μm, and the system resolution in the transverse direction was about 1 μm. It should be noted that the limitation of the transverse size is partly due to the averaging over the source projection.

Proportionality of the height of peaks to the double phase shift $2\varphi = 4\pi\delta\, t/\lambda$ linearly increasing with the longitudinal size *t* is clearly observed in Fig. 3, which must be observed in the Zernike phase contrast method as well. At the same time, the calculation has shown that the background subsidence effect, which is especially notable with an increase in the longitudinal size of objects, takes place as well in addition to the expected image contrast enhancement of objects with an increase in the phase introduced by them. This behavior is apparently caused by the principle of conservation of integral intensity. Note that a decrease in the intensity around the images of objects did not directly follow from the known equations illustrating the Zernike concept. It is purely the diffraction effect that cannot be explained in the framework of the approximate theories of the Zernike phase contrast method. Thus, computer simulation shows that the Zernike concept is only the suggestion of the contrast enhancement effect and the real mechanism of the image formation is most complex.

The next important problem was to determine how the image quality depends on the object position at the lens aperture. For this purpose a set of objects arranged along the aperture was simulated in the work. The objects had different shape and thickness and shifted the phase in different ways that allowed us to observe a whole specter of different situations by one graph. The calculated intensity distribution (Fig. 4a) was normalized to the source intensity value without object; therefore, in the ideal case, the height of intensity peaks on the level of background should be double phase induced by objects. For more suitable comparison the exact values of double phases are shown as well (Fig. 4b), and one can observe the shape and thickness of the simulated objects.

As follows from calculations and Fig. 4, a refracting lens most qualitatively images the objects arranged in the central part of aperture. When the object is removed from the center of the aperture, the quality of its image notably decreases and proportionality between the object phase and image contrast disappears as well. In addition, information about the shape of objects is lost, namely, the images of the samples shifted from the center of aperture and having initially rectangular configuration take the form of trapeziums. The image distortion at the aperture edges is related to the features of the structure of X-ray refracting lenses. Since these lenses are concave and have rather small radius of curvature, the absorption effect is especially strong at the edges, in the thickest lens areas. It is easy to understand that the beams scattered at a small angle and transmitted virtually straight carry the main information about the object. Therefore, the strong absorption at the aperture edges leads first of all to the loss of information about the objects removed from the center of aperture, whereas the central objects are virtually imaged without distortions.

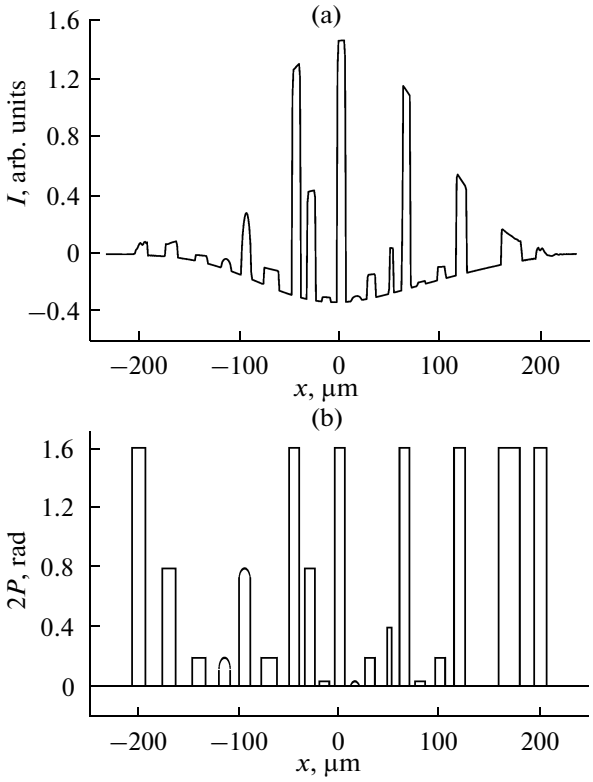


**Fig. 4.** (a) Distribution of the difference in radiation intensities with and without objects in the Zernike method with a refracting lens for a series of different objects distributed over the lens aperture. (b) Profile of the double phase shift formed by the considered objects.

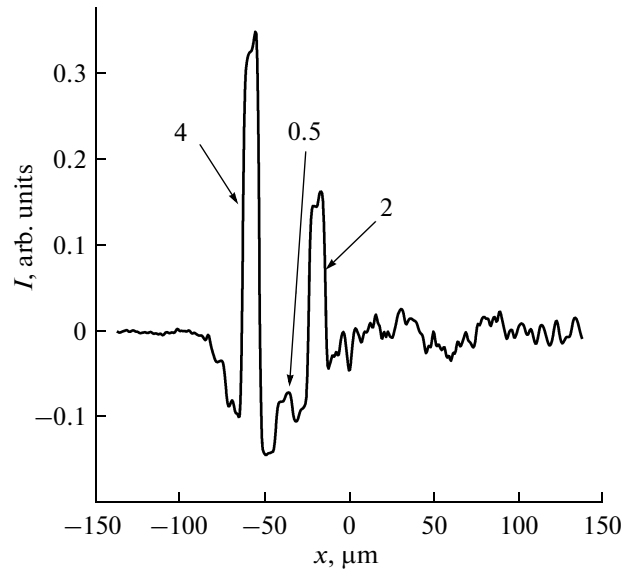


**Fig. 5.** Spatial distribution of the difference in intensities with and without objects when a zone plate is used in the Zernike scheme. The objects were three slugs with rectangular cross section and different longitudinal sizes $d$. The $d$ values in μm are written by the curves.

## 5. THE CALCULATION RESULTS FOR THE SCHEME WITH ZONE PLATE

The scheme for calculations of the Zernike phase contrast with a zone plate is shown in Fig. 2. As in the previous section, the sample was placed at the double focal distance from a zone plate and the inversed image of the sample is formed without enlargement at the double focal distance. In the work a gold zone plate was considered with the following parameters: number of zones $N = 400$, aperture $A = 160$ μm, and focal distance $F = 16$ cm.

The characteristic feature of the given scheme is that a zone plate has many orders of focusing, in contrast to a refracting parabolic lens. The definite part of the initial beam carrying itself one or another portion of its intensity is focused in each order. Even for the perfect zone plate shifting the wave field phase in zones by $\pi$, the first order is directly responsible for the image formation in the scheme and has 40% of the total intensity. The remaining 60% of radiation does not come to the focus of the first order and does not directly participate in the formation of the resulting image pattern of objects. This radiation comes also to a detector and interferes with the basic wave perniciously effecting on the image quality. Therefore, in the case of the zone plate, the standard Zernike scheme does not allow us to observe phase objects.

In the given work, a perfect zone plate (ZP) without zero order is considered. To exclude the effect of the minus first order of focusing on the image, the investigated object was placed beyond the optical axis rather than in the center (Fig. 2, upper). In this case, as is shown in Fig. 2, an inverse image of the object in the first order of focusing is formed in the lower part of the ZP aperture, whereas a nonfocused image in the minus first order appears in the upper part of the aperture and beyond the aperture. Thus, they do not overlap.

There is another reason to decay the image: the overly high degree of the incident beam coherence. It is known that a similar level of coherence leads frequently to the formation of destructive speckles [10]; therefore, the phase noise is specially formed in some experiments, for example, by virtue of rotating diffusers. To suppress spurious interference of different orders the averaging of calculated pattern with the Gaussian function of the definite half-width was used in the given work. The optimal half-width was $S = 2$ μm. Note that the lenses have no different orders of focusing and the required degree of averaging is smaller.

The use of the above-indicated modification resulted in the fact that the image contrast increased and phase objects became visible, although the image resolution obtained in the scheme with a zone plate is not so high as with a lens. In this case the proportionality of the height of the peak to the double phase of the object and the background subsidence providing the conservation of the integral intensity are observed as in the use of lens. The spatial distribution of the difference in the intensities with objects and without them is shown in Fig. 5 when a zone plate was used in the Zernike scheme. The objects were three slugs with

rectangular cross section and different longitudinal sizes, 0.5, 2, and 4 μm.

## 6. CONCLUSIONS

It has been shown that both a refracting parabolic lens and a zone plate can be successfully used as objects in the Zernike phase contrast method for hard X-ray radiation. Each of these X-ray-optical devices has own features, advantages, and disadvantages. A refracting lens reconstructs most effectively the structure of the objectives arranged in the central part of aperture, whereas the samples at the periphery are not virtually imaged. The minimal longitudinal and transverse sizes of silicon objects that can be observed by the lens were 0.1 and 1 μm, respectively. A zone plate after the Zernike method modification allows the reconstruction of the structure of objects as well; however, it has lower resolution. In a whole, the Zernike method shows better possibilities in the X-ray range than the usual phase contrast technique. According to the results of the carried-out work, we can conclude that the method of the image formation of microobjects by the Zernike scheme in the hard X-ray range is promising and requires further investigation. In particular, it is worthwhile to study the possibilities of its application, not only for existing synchrotron sources, but also for further X-ray free electron laser sources.

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