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Simulation of image formation using compound X-ray zone plates

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ABSTRACT

In this paper, we consider the correlation between the resolution of a Fresnel zone plate and the width of its outermost zone. Obtaining an image of an X-ray source using multi-order zone plates is discussed. It is shown that the resolution of a conventional Fresnel zone plate can be improved by a factor of 10 by designing a compound zone plate with six operative orders, with the width of the outermost zone remaining unchanged. In this case, the efficiency of focusing the X-rays into an image is slightly less than 4 per cent. Note that the efficiency attained is 1.5 times that of a conventional third-order Fresnel zone plate. In addition, the resolution of the compound zone plate is 3.05 times that of a conventional second-order Fresnel zone plate.

1. Introduction

Zone plates (ZP) are widely used in X-ray microscopy [1–4]. Fresnel ZPs are used as imaging optics due to their simplicity of manufacturing and small thickness, which is the necessary quality for X-ray zone plates, because hard X-ray radiation is absorbed in most materials. The thickness of the ZP is limited by the thickness of the material required to form a phase shift of π between different zones and the thickness of a substrate layer which provides the necessary mechanical strength. The spatial resolution of a ZP working in the first transmitted diffraction order is defined by the outermost zone width. For example, lines of width of up to 38 nm have been experimentally resolved using an optical system composed of two zone plates [2]. The outermost zone width of the objective zone plate had a thickness of 50 nm. An optical system containing two identical zone plates of radius 37.75 μm and outermost zone width 20 nm synthesized in gold was experimentally investigated in Ref. [5]. Lines with a minimal width of 160 nm were experimentally resolved using such zone plates. It was numerically shown in Ref. [6] that a zone plate with a staggered order of zones can focus hard X-ray radiation. Its outermost zone width was equal to 350 nm, and a focal spot with a diameter of 2 mm was numerically obtained. The best resolution in an X-ray microscope was demonstrated in Refs. [7,8]. A zone plate with the outermost zone width of 12 nm has enabled achieving a 12-nm resolution.

As seen from [1–8], the main challenge in obtaining higher resolution is associated with the technical feasibility to create a zone plate with the minimal zone width. The wavelength of the hard X-rays is much less than the zone width (tenths of

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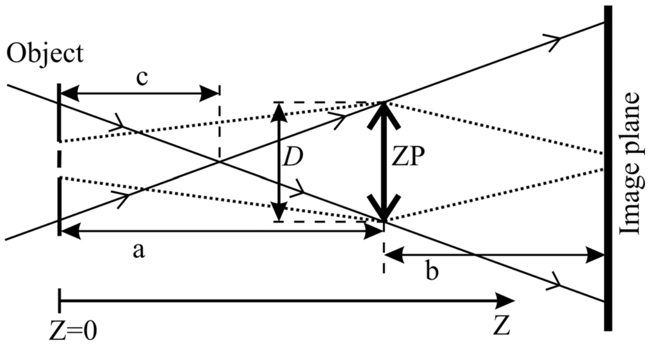

Fig. 1. Schematic diagram of the problem under study.

nanometer) and does not affect the resolution. Because the Fresnel ZP is a binary diffraction element, it forms spurious focuses in the 3-d, 5-th, 7-th diffraction orders, and so on [6,9]. The diameter of the spurious focal spots is considerably smaller than that of the main focal spot in the first diffraction order [6,8], thus enabling obtaining a ZP with higher resolution [10].

A concept of the compound zone plate was first proposed by Simpson in Ref. [10]. In an attempt to alleviate fabrication difficulties, many strategies were proposed [11,12]. Particularly, Xie et al. [11] proposed a compound zone plate, central part of which is realized as a photonic crystal. A focal spot with FWHM = 51.1 nm for a minimal hole diameter of 100 nm was obtained. And in Ref. [12] differential-interference-contrast digital in-line holography microscopy was investigated. A compound ZP working in the 1-st and 3-d diffraction orders was experimentally investigated in Ref. [13], its outermost zone width was equal to 50 nm. This zone plate was able to image periodical lines with a width of 25 nm. Furthermore, Keskinbora et al. [14] created a ZP with the outermost zone width of 100 nm. Using such a zone plate operating in the third diffraction order for scanning microscopy, diffraction grating lines of width 28.5 nm were resolved. Note that the experiments were carried out without the rigorous numerical modeling of image formation by a multiorder compound zone plate.

In this work, we look into the possibility to use compound zone plates operating in several diffraction orders as imaging X-ray optics, attaining a spatial resolution which significantly exceeds that of a conventional ZP that operates in the first diffraction order and has the same width of the outermost zone. Rigorous numerical modeling using integral methods is a complex computational problem which requires the use of high-performance computers, long run times [15] and is carried out rarely. The propagation of X-rays in free space can be simulated using a variety of techniques. The most popular paraxial approximation is based on the Fresnel integral. In this work, the numerical modeling was conducted using a more general Rayleigh-Zommerfeld integral [9]. We have chosen it because, on the one hand, its accuracy is not worse than that of the Fresnel integral and, on the other hand, we could use a faster algorithm for it.

2. Numerical modeling

Shown in Fig. 1 is a scheme of the problem under study.

A converging X-ray beam falls on an object and then achieves a zone plate forming a magnified image at the output plane. The wavelength of the X-ray beam is $\lambda = 0.229$ nm. It was chosen so because it is the wavelength emitted by an X-ray tube with a chromium anode. A converging incident beam is considered, because it diverges after an object plane enough, thus reducing the negative influence of the beam on the image contrast. Such a converging beam can be formed, for example, by a capillary Kumakhov lens [16,17], a sphere set located on the optical axis, or by another zone plate [18]. Another advantage of the converging incident beam is that such a beam can improve efficiency because the radiation is distributed over the entire ZP working area, and no additional blocking baffle is needed.

The parameters of the ZP working in the first order have been chosen to be suitable for the further manufacture of the ZP by electron lithography. The outermost zone width (a half period) is $\Delta r = 205$ nm.

At the given wavelength, the intensity of X-rays having propagated over 30 cm reduces two-fold, a minimal-length optical scheme and a short-focus ZP should be used. Thus, for a ZP of diameter $D = 200$ μm, a focal length of $f = 18$ cm was chosen. The relief height of $h = 1.8$ μm must be used for a zone plate made of silver (the refraction index of silver for the given wavelength is $n = 1 - 6.38 \times 10^{-5} - 1.13 \times 10^{-5} i$). Using a smaller microrelief height will result in less aspect ratio, simpler design, but will decrease intensity in the image. Although the proposed aspect ratio (AR) of 8.7 seems to be fairly high, there have been techniques for attaining much higher aspect ratios of Fresnel zone plates for hard X-rays. For instance considering that in Ref. [19] AR = 21 was reported, the value of AR = 8.7 proposed in this work does not seem to be unattainable. For a 5× magnification considered in this work, the optical scheme parameters are $a = 0.216$ m, $b = 1.08$ m for the given focal length. To provide a sufficiently high resolution of the incident field phase it is appropriate to assume the step of a discretization grid to be equal to 0.13 μm, with the entire ZP being 1539 × 1539 pixels. If the ZP under study is used for obtaining a greater magnification, the optical scheme will become longer which can negatively affect the use of the optical scheme in the experiments.

The pixel size of 0.13 μm may appear to be too large for accurate calculations. However, it has been numerically demonstrated [15] that pixels considerably larger than the wavelength can be used without adversely affecting the calculation