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Technical Notes

Numerical design of in-line X-ray phase-contrast imaging based on ellipsoidal single-bounce monocapillary

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ABSTRACT

A new device using an ellipsoidal single-bounce monocapillary X-ray optics was numerically designed to realize in-line X-ray phase-contrast imaging by using conventional laboratory X-ray source with a large spot. Numerical simulation results validated the effectiveness of the proposed device and approach. The ellipsoidal single-bounce monocapillary X-ray optics had potential applications in the in-line phase contrast imaging with polychromatic X-rays.

1. Introduction

X-ray phase-contrast imaging is appropriate to observe the object composed of light element [1,2]. In theory, the X-ray phase-contrast imaging can distinguish the boundary with the density fluctuation of $0.3-2.0\ \text{kg m}^{-3}$, and its spatial resolution can reach 1 μm. For X-ray phase-contrast imaging, a high intensity source which can provide coherence light is needed in order to obtain the interference. It is generally acknowledged that a synchrotron radiation source is appropriate. But as a multi-disciplinary large-scale research platform, the synchrotron radiation source is hardly used widely in X-ray phase-contrast imaging because this complex equipment is expensive and equipment-hour is limited. In 1996, Wilkins puts forward an in-line X-ray phase-contrast imaging method of using a micro-focus polychromatic X-ray source to realize X-ray phase-contrast imaging, which only has the requirement of high spatial or lateral coherence of the X-rays [3]. The key of this method is using the micro-focus polychromatic X-ray source to get the X-rays with high spatial coherence. This method makes it possible to perform the X-ray phase-contrast imaging in an ordinary laboratory. In order to analyze the effect from the partially coherence of the X-rays on the in-line X-ray phase-contrast imaging quality, Paganin and Nugent discuss this effect by using a transport-of-intensity Equation [4], and Hong Yu et al. present a general treatment of X-ray image formation by direct Fresnel diffraction with partially coherent hard X-rays [5].

Some micro-focus X-ray source now can meet the requirement for the in-line X-ray phase-contrast imaging with polychromatic X-rays. However, such micro-focus source is very expensive, and moreover, its power is low. This is not helpful for promoting the researches on X-ray phase-contrast imaging in the ordinary laboratory. There are some X-ray focusing optics, such as Schwarzschild objectives, zone plates, multilayer Laue lenses, refractive optics and the capillary X-ray optics lens, which can effectively implement the conversion from the X-ray source with a large spot to the micro-focus source [6]. However, not all of such optics is suitable for being used in the ordinary laboratory for the in-line X-ray phase-contrast imaging with polychromatic X-rays. For example, Schwarzschild objectives are limited to the EUV region. Bent crystal optics can only focus the monochromatic X-rays into a single focal spot. Although zone plates which are easiest to make for soft X-rays with high aspect ratio have been demonstrated for hard X-rays, however, with a conventional source, only a small collection angle can be achieved because the outer diameter of the zone plates optics is quite small, so synchrotron sources are typically required to provide sufficient flux. Similar restrictions tend to limit both refractive optics and multilayer Laue lenses to synchrotron sources [6].

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Capillary X-ray optics lens can be used to collect the X-rays in a wide energy band from a relatively large source angle, and have wild application prospect for in-line X-ray phase-contrast imaging [5]. Capillary X-ray optics can be divided into two major categories of polycapillary X-ray optics and monocapillary X-ray optics. The polycapillary X-ray optics is also named with Kumakhov lens are combined with a large number bundles of hollow glass fibers [7], and they are able to focus X-rays into a focal spot with diameters of tens of micrometers. The monocapillary X-ray optics, which is made of a single hollow glass tube, can focus X-rays into micron and even submicron focal spot [8]. When the polycapillary X-ray optics is used for the in-line phase contrast imaging, the 'hexagon' pattern background caused by the walls between the compound polycapillaries will affect the imaging quality [5,9]. Moreover, the polycapillary X-ray optics is not imaging optics, and its focal spot size varies at different energies of the X-rays [10]. In other words, although the polycapillary X-ray optics can focus the polychromatic X-rays into the same focal spot position, the X-rays with different energies have different focal spot sizes at this same focal spot position of the polycapillary X-ray optics. This is not helpful for the in-line phase contrast imaging.

In this paper, in order to avoid problems from the polycapillary X-ray optics, an ellipsoidal single-bounce monocapillary X-ray optics (ESBMCXRO) was proposed to be used to focus the X-rays from conventional X-ray source with a large spot for performing the in-line phase contrast imaging with polychromatic X-rays. The performances of the application of the ESBMCXRO in the in-line phase contrast imaging were simulated.

2. Principles of simulation

2.1. Algorithm for ESBMCXRO

The distribution of X-ray intensity in the focal spot of the ESBMCXRO was simulated by the following method [11]. As shown in Fig. 1, X-rays leaving the point source at (x_s, y_s) are reflected once on an infinite small ellipsoidal capillary surface at angular position ϕ and focused to point (x_i, y_i). For an infinite small ellipsoidal reflection surface, the image position can be given as:

$$x_i = -M(x_s \cos 2\phi + y_s \sin 2\phi),\quad y_i = M(y_s \cos 2\phi - x_s \sin 2\phi) \quad (1)$$

where $M = F_2/F_1$, is the magnification, and other symbols are shown in Fig. 1.

Using the substitutions $x_{s,i} = r_{s,i} \cos \theta_{s,i}$, $y_{s,i} = r_{s,i} \sin \theta_{s,i}$ to rewrite image equations as:

$$r_i = M r_s,\quad \theta_i = \pi - (\theta_s - 2\phi) \quad (2)$$

It is convenient to use capillary azimuth angular coordinate ϕ to represent the image brightness angular dependence. As long as $\Delta l \ll F_1, F_2$, where Δl is the length of a section of capillary, the image brightness (flux/solid angle/area) B_i is related to source brightness B_S by $B_i(r_i, \theta_i, \phi) = B_s(r_i/M, 2\phi - \theta_i)$, and B_s is assumed to have up-down and right-left symmetry. Assuming y_1 and y_2 are the radius

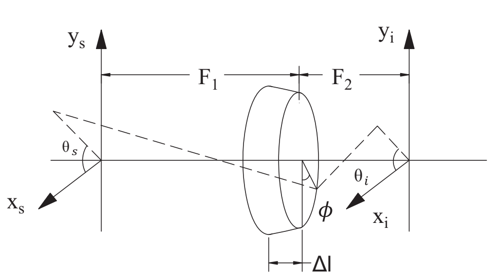

Fig. 1. Diagram for ESBMCXRO of focusing X-rays.

at larger and smaller end of this small capillary segment, respectively, the photon flux density, ΔF_i, from this small capillary segment at image plane will be $(y_1;\ y_2 \ll F_1;\ F_2)$,

$$\Delta F_i(r_i, \theta_i) = (f/F_2^2)\oint B_i(r_i, \theta_i, \phi)d\phi = (2\pi f/F_2^2)\overline{B}_S(r_i/M) \quad (3)$$

where $2\pi f = \pi(y_1^2 - y_2^2)$ is the radiation interception area by capillary length Δl, and $\overline{B}_S$ is the azimuthal angular average of B_S. Eq. (3) explains mathematically that the image flux is angularly symmetric, i.e., $F_i(r_i, \theta_i) = F_i\ (r)$. Summation of Eq. (3) over the whole capillary length gives the image flux profile from the capillary.

2.2. Basics of in-line X-ray phase-contrast imaging

When the X-rays irradiate on the object, the interactions between the object and X-rays include absorption, scattering and refraction. The refraction causes tiny changes of the direction of propagation, which contains the information about the variation of refractive index of the object.

The X-ray refractive index n characterizing the optical properties of an object can be expressed as $n = 1 - \delta - i\beta$, in which δ is the decrement of real part of the refractive index, characterizing the phase shifting property, while the imaginary part β characterizes the absorption property of the object.

With coherent light source, when the wave-front passes through the pure phase sample with no absorption, phase difference inevitably emerges at the wave-front, which results from the variation of δ, i.e., wave-fount distortion happens. The distortional wave can be measured by the intensity change. However, because X-ray refraction angles are usually quite small (a few arc seconds), the measurement of the refraction effect requires extremely sophisticated instruments and effective means. The lateral coherence length is $d_\perp = \lambda d/\sigma$, where σ is the source size, and d is the distance between the source and the observing place. Hence, the smaller σ source and the larger d can provide a higher spatial or lateral coherence. However, when the distance increases, the intensity of X-rays will become weak, and the output intensity given by micro-focal spot source is relatively limited. So the d and σ are two significant parameters, and they can be adjusted to achieve both the acceptable spatial coherence and the intensity.

Under partially coherent condition, the intensity distribution of the in-line X-ray phase-contrast imaging on image plane is given by Ref. [5] by following.

For a pure phase object, under the paraxial approximation, the image intensity distribution $I(u, v)$ in the spatial frequency domain is

$$I(u,v) = c\frac{\rho^2}{l^2}\left\{\delta\left(\frac{z}{f}u, \frac{z}{f}v\right) + \frac{2J_1(\gamma)}{\gamma} \times 2\sin\left[\pi\lambda z\left(\frac{z}{f}u^2 + \frac{z}{f}v^2\right)\right]\Psi\left(\frac{z}{f}x, \frac{z}{f}y\right)\right\} \quad (4)$$

where c is constant, and $1/f = 1/z + 1/l$, l is source to object plane distance, z is object plane to phase distance, ρ is the radius of the light source, λ is the wavelength, $J_1(\gamma)$ is the first-order Bessel function, $\gamma = 2\pi\rho/l\sqrt{u^2+v^2}$ $\Psi((z/f)x, (z/f)y)$ is the Fourier transform of the phase difference φ for a ray path through an object.

Ignoring background, the normalized optical transfer function (OTF) is

$$H(u,v) = \frac{2J_1(\gamma)}{\gamma} \times \sin\left[\pi\lambda z\left(\frac{z}{f}u^2 + \frac{z}{f}v^2\right)\right] \quad (5)$$

Suppose $l \to \infty$, we get $f = z$, $\gamma = 0$, and then the normalized OTF of fully coherent X-rays is

$$H(u,v) = 2\sin\left[\pi\lambda z(u^2+v^2)\right] \quad (6)$$

When the space frequencies are small enough, $J_1(X) \approx X/2$, $\sin X \approx X$. Then,

$$H(u,v) = 2\pi\lambda z \times z/f(u^2+v^2) \quad (7)$$