

X-RAY OPTICS

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Simulation of grazing-incidence coherent imaging

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***Abstract.* A method is proposed for simulating optical object images formed by oblique or grazing-incidence coherent beams. The theoretical approach relies on the solution of a parabolic equation, which generalises the Fresnel integral. Our numerical results are given for experimental conditions close to those realised when use is made of modern soft X-ray lasers. The newly developed method may also be employed to simulate X-ray imaging systems developed around synchrotron and free-electron laser beams.**

Keywords: *X-ray optics, grazing incidence, imaging, parabolic wave equation.*

1. Introduction

The development and availability of laboratory-scale as well as of large-scale X-ray laser facilities [1, 2] have generated considerable recent interest in coherent methods of obtaining and analysing X-ray images. Important advantages of employing coherent beams in microscopy and microanalysis are the possibilities to reconstruct the wave field at the object without the use of optics and to measure the phase of the field in the image plane [3, 4].

At the present time, the wavelength range best mastered by X-ray lasers is the 10 – 40 nm range*. All materials exhibit an extremely low transmittance in this spectral range, and layer thicknesses may not exceed tens of nanometres. As a consequence, primary emphasis is placed on the methods for studying objects in reflected beams (Fig. 1). As the wavelength becomes shorter, the grazing angle θ must be made smaller to obtain a sufficiently high reflection coefficient.

When an object is illuminated by a coherent beam, the use of an optical system between the object and the detector is not obligatory. However, the total reconstruction of the wave fields (including the phase) at the object (u_0) and the detector (u) has to rely on algorithms that establish the relationship between u_0 and u. In the illumination of the object along the normal to its surface ($\theta = \pi/2$, Fig. 1), the relationships required for analysing the transmitted or reflected beams are defined by the Fresnel integral. In the case of oblique radiation incidence on a specimen, especially for small angles θ, which are of interest for investigations in the X-ray domain, the applicability of the Fresnel integral is not substantiated.

In the present work we consider several properties of the coherent beam propagating on oblique reflection from an object that are required for determining the fields at the detector and for solving problems involving the field phase reconstruction in the image plane.

2. Source function for normal and oblique radiation incidence on an object

The principal instrument of simulations in incoherent optics is the Fresnel integral. It defines the wave field $u(x, z)$ by its value $u_0(s)$ in plane S (Fig. 1):

$$u(x,z) = \sqrt{\frac{k}{2\pi i z}} \int_{-\infty}^{\infty} u_0(s)\,\mathrm{d}s \exp\left[i\frac{k(x-s)^2}{2z}\right]$$

$$= \int_{-\infty}^{\infty} K_0(x,z,s)\,u_0(s)\,\mathrm{d}s, \quad (1)$$

$$K_0(x,z,s) = \sqrt{\frac{k}{2\pi i z}} \exp\left[i\frac{k(x-s)^2}{2z}\right],$$

where $K_0(x, z, s)$ is the source function, which is the field induced by the distribution $u_0(s, s') = \delta(s - s')$. For brevity of notation, we restricted ourselves to the two-dimensional case. The applicability condition for expression (1) is the perpendicularity of object plane S, in which the field $u_0(s)$ is defined, to the direction of beam propagation, which we assume to be horizontal. When this is not the case, i.e. the plane S makes an angle $\theta \neq \pi/2$ with the z axis, as shown in [8], instead of $K_0(x, z, s)$, in expression (1) one must use the source function

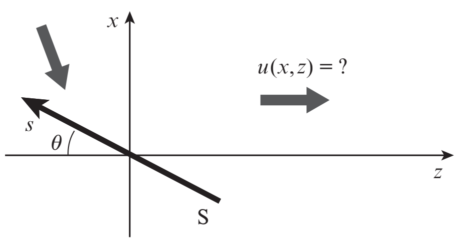

Figure 1. General schematic of image formation with an obliquely incident beam.

*Operating in the $\lambda \sim 1$ Å wavelength region is the Linac Coherent Light Source (LCLS) [5]. Several other facilities intended for operation in this or softer spectral regions are under construction or design [6, 7].

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$$K(x,z,s,\theta) = \left(\frac{x-s'}{z'}\cos\theta + \sin\theta\right)K_0(x,z',s'),\ \ x > -z\tan\theta,$$
$$K(x,z,s,\theta) = 0,\ \ x < -z\tan\theta, \tag{2}$$

where $z' = z + s\cos\theta$; $s' = s\sin\theta$.

Expressions (1) and (2) are the solutions of the parabolic wave equation

$$2\mathrm{i}k\frac{\partial u}{\partial z} + \frac{\partial^2 u}{\partial x^2} = 0, \tag{3}$$

which describe the fields propagating from the plane object illuminated by a coherent beam at an angle $\theta \leqslant \pi/2$. Therefore, for arbitrary θ the analogue of integral (1) is of the form

$$u(x,z) = \sqrt{\frac{k}{2\pi\mathrm{i}}}(x\cos\theta + z\sin\theta)$$
$$\times\int_{-z/\cos\theta}^{\infty}\frac{u_0(s)\,\mathrm{d}s}{(z+s\cos\theta)^{3/2}}\exp\left[\mathrm{i}\frac{k(x-s\sin\theta)^2}{2(z+s\cos\theta)}\right], \tag{4}$$
$$x > -z\tan\theta.$$

It will be assumed that the object is bounded, its right edge is located at $s = 0$, and that optical elements are accommodated in the domain $z > 0$, where the field according to expression (4) is defined by the following integral:

$$u(x,z) = \sqrt{\frac{k}{2\pi\mathrm{i}}}(x\cos\theta + z\sin\theta)$$
$$\times\int_{0}^{\infty}\frac{u_0(s)\,\mathrm{d}s}{(z+s\cos\theta)^{3/2}}\exp\left[\mathrm{i}\frac{k(x-s\sin\theta)^2}{2(z+s\cos\theta)}\right],$$
$$x > -z\tan\theta,\ \ z > 0, \tag{5}$$
$$u_0(s) = 0 \text{ при } s < 0. \tag{6}$$

Formulas (5) and (6) may be employed to simulate the formation of the images of inclined objects of finite size. However, they possess an obvious disadvantage. The field (5) is defined only within some angle, this field being equal to zero on the angle side $x = -z\tan\theta$ (i.e. in the object plane) for $s < 0$. In reality the field is determined by diffraction, which accompanies the beam propagation from the object into the domain $z > 0$.

The following approach seems to be more natural and physically justified. The exact solution (4) is used to determine the field in the vertical plane $z = 0$, which passes through the right edge of the object. This causes no difficulties in the domain $x > 0$. At the same time, according to expression (4) the field is undefined for $x < 0$. In the absence of any additional indications related to experimental condition, we put it equal to zero. Therefore, for $z = 0$ we have

$$u(x,z=0) = \sqrt{\frac{k}{2\pi\mathrm{i}\cos\theta}}\,x$$
$$\times\int_{0}^{\infty}\frac{u_0(s)\,\mathrm{d}s}{s^{3/2}}\exp\left[\mathrm{i}\frac{k(x-s\sin\theta)^2}{2s\cos\theta}\right],\ \ x > 0, \tag{7}$$
$$u(x,z=0) = 0,\ \ x < 0.$$

Next, to calculate the field in the right half-space $z > 0$, we take advantage of the Fresnel integral (1) with the initial distribution defined by expression (7). We perform the integration (see, for instance, Ref. [9]) to obtain

$$u(x,z) = \frac{1}{2\pi}\frac{\exp[\mathrm{i}kx^2/(2z)]}{\sqrt{z\cos\theta}}$$
$$\times\int_0^{\infty}\frac{u_0(s)\,\mathrm{d}s}{s^{3/2}A}\exp\left(\mathrm{i}k\frac{s\sin^2\theta}{2\cos\theta} + \zeta^2\right)F(\zeta), \tag{8}$$

$$A = \frac{1}{s\cos\theta} + \frac{1}{z},\ \zeta = B\sqrt{\frac{k}{2\mathrm{i}A}},\ B = \tan\theta + \frac{x}{z},$$
$$F(\zeta) = \exp(-\zeta^2) + \sqrt{\pi}\,\zeta[1 + \Phi(\zeta)],$$
$$\Phi(\zeta) = \frac{2}{\sqrt{\pi}}\int_0^{\zeta}\exp(-t^2)\,\mathrm{d}t. \tag{9}$$

Therefore, there are two approaches to the calculation of fields about objects illuminated by obliquely incident beams. They are represented by formulas (5), (6) and (8), (9), respectively. The former defines the field only within the angle (5), while the latter enables determining the wave field in the half-space $z > 0$. In essence, the employment of formulas (8), (9) in lieu of formulas (5), (6) signifies a more exact inclusion of diffraction at the edge of the object.

It is easily verified that formulas (5), (6) and (8), (9) result in different field distributions not only in the near-field region, but also in the far-field region. In the former case, in particular, for the source function in the far-field region we have [10]

$$K(x,z,s,\theta) = \sqrt{\frac{k}{2\pi\mathrm{i}z}}\left(\frac{x}{z}\cos\theta + \sin\theta\right)$$
$$\times\exp\left[\mathrm{i}\frac{kx^2}{2z} - \mathrm{i}\frac{kx}{z}\left(\frac{x}{z}\cos\theta + \sin\theta\right)s\right]. \tag{10}$$

For $\theta = \pi/2$ this expression transforms naturally into the source function corresponding to the Fraunhofer limit of the Fresnel integral (1).

As discussed in the foregoing, the inclusion of the finiteness of the object calls for a more exact treatment of diffraction beyond its edge (in the domain $z > 0$). This signifies that use should be made of expressions (8), (9) instead of expressions (5), (6). We put $x, z \gg s$ to obtain

$$K(x,z,s,\theta) = \frac{1}{2\pi}\left(\frac{x}{z}\cos\theta + \sin\theta\right)\sqrt{\frac{\cos\theta}{zs}}$$
$$\times\exp\left[\mathrm{i}\frac{kx^2}{2z} - \mathrm{i}\frac{kx}{z}\left(\frac{x}{z}\cos\theta + \sin\theta\right)s\right]F(\zeta), \tag{11}$$
$$\zeta = \left(\tan\theta + \frac{x}{z}\right)\sqrt{\frac{ks\cos\theta}{2\mathrm{i}}}.$$

One can see that expression (11) transforms into expression (10) when $\zeta \gg 1$. However, for $\zeta \ll 1$, i.e. in the case of illumination at a small angle, low apertures, and objects of small size, the difference between formulas (11) and (10) may be significant and the effects associated with the finiteness of the object should be taken into account for oblique illumination.

So, we have considered two approaches to the simulation of the coherent images of inclined objects of finite size. They are represented by formulas (5), (6) and (8), (9). The former approach is computationally simpler; however, it is less exact in the treatment of diffraction at the edge of the object.

3. Simulation results

The approach described by formulas (8), (9) was implemented in the form of programmes simulating the formation of coherent images of obliquely illuminated objects by optical systems. We outline the results in the case when the optical system is an ideal lens with a finite numerical aperture NA = $\sin\varphi$ (Fig. 2). In the field equations, the lens is described by a thin phase screen

$$T(x) = \exp\left(-\frac{ikx^2}{2f}\right) \tag{12}$$

of diameter $2f\tan\varphi$, where f is the focal distance. The coherent monochromatic radiation is obliquely incident on the object of size l, which is located in plane S at a distance $a = 2f$ on the left of the lens. The image is constructed in the conjugate plane S′, which intersects the optical axis at a distance $a' = 2f$ from the lens.

At the first stage, proceeding from the initial field $u_0(s)$, we calculated the wave field in the plane $z = 0$. In accordance with the approach outlined in Section 2, for $x > 0$ there applies formula (7), and for $x < 0$ we put $u(x) = 0$. The subsequent calculations of the field at the lens and in the image plane were carried out by Fresnel formula (1). The wavelength and other parameters were selected in such a way as to correspond to the experimental conditions involving laboratory X-ray lasers [1]: $\lambda = 10$ nm, $l = 40$ μm, $\theta = 90°$ and 1°, NA = 0.2 and 0.06. The simulation results given in Fig. 3 suggest that the similarity between the object and the image is retained down to very small grazing angles ($\theta = 1°$) and begins to break down when the numerical aperture is decreased from 0.2 to 0.06. Qualitatively, this is consistent with the diffraction-limited estimate $\delta \approx \lambda/(\mathrm{NA}\sin\theta)$.

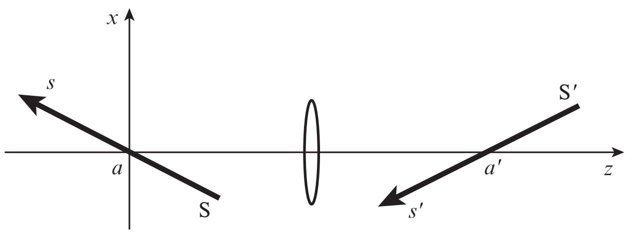

Figure 2. Imaging with an ideal thin lens. The object is located in plane S and the image in plane S′.

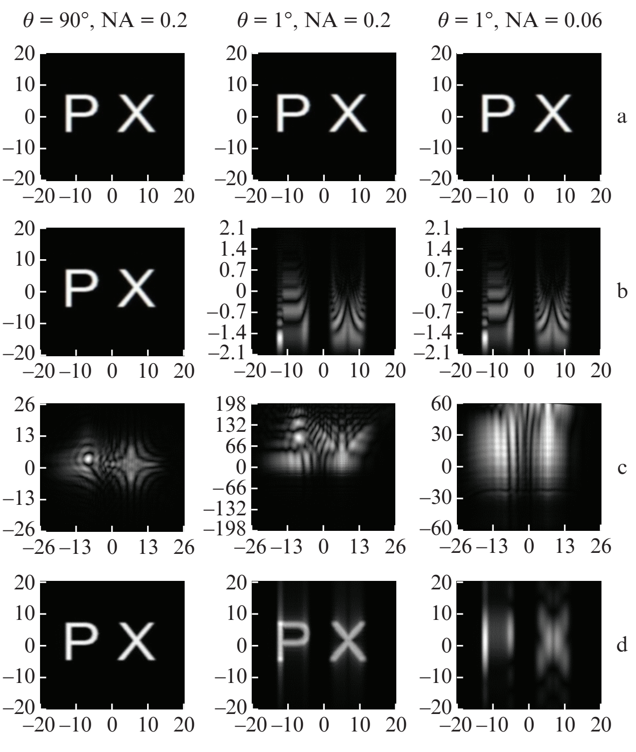

Figure 3. Spatial field amplitude distributions: at the initial object (a), in the intermediate plane (b), at the lens (c), the final image (d). The scales on axes are in micrometres.

4. Conclusions

Therefore, we have developed and tested a method for the simulation of optical systems which image objects illuminated by coherent grazing-incidence beams. The corresponding experiments hold interest for X-ray lasers. When normal incidence of the laser beam onto a detector is required, the experimental setup may be supplemented with a diffraction grating or an asymmetric crystal placed after the optical system.

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