Optics Communications 410 (2018) 130–141

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

X-ray simulations method for the large field of view

I.A. Schelokov [a,b,*], M.V. Grigoriev [a], M.V. Chukalina [b,a], V.E. Asadchikov [b]

[a] Institute of Microelectronics Technology and High Purity Materials, Russian Academy of Sciences, Chernogolovka, Moscow Region, Chernogolovka, Academician Ossipyan str, 6, 142432, Russia

[b] Shubnikov Institute of Crystallography, Russian Academy of Sciences, Leninskii pr. 59, Moscow, 119333, Russia

ARTICLE INFO

Keywords:
X-ray optics
Ambiguity function
Talbot interferometry

ABSTRACT

In the standard approach, X-ray simulation is usually limited to the step of spatial sampling to calculate the convolution of integrals of the Fresnel type. Explicitly the sampling step is determined by the size of the last Fresnel zone in the beam aperture. In other words, the spatial sampling is determined by the precision of integral convolution calculations and is not connected with the space resolution of an optical scheme. In the developed approach the convolution in the normal space is replaced by computations of the shear strain of ambiguity function in the phase space. The spatial sampling is then determined by the space resolution of an optical scheme. The sampling step can differ in various directions because of the source anisotropy. The approach was used to simulate original images in the X-ray Talbot interferometry and showed that the simulation can be applied to optimize the methods of postprocessing.

1. Introduction

Simulation is a powerful instrument for scientific research in various fields and solution of numerous engineering problems. In the X-ray wave range, simulation has some specific features. On the one hand, an extremely short wavelength enables studies of micro- and nanoscale objects. On the other hand, a high penetration ability of X-rays is of interest for diagnostics of macroobjects, e.g. medical radiographs or weld seams on tubes. A question arises whether so much differing interests can be combined in optical simulation, whether the Angstrom-range wavelength can be involved in studies dealing with objects of millimeter, centimeter, decimeter or even larger scales. Here we present a method for X-ray simulations which can readily modify the numerical scheme to meet the requirements of a given task.

Simulations of optical schemes with an incoherent radiation source actually consist in calculating the following integral expression [1]

$$I\left(x_{\mathrm{det}}, y_{\mathrm{det}}\right) = \int I\left(\xi,\eta\right)\left|K\left(\xi,\eta; x_{\mathrm{det}}, y_{\mathrm{det}}\right)\right|^2 d\xi d\eta \tag{1}$$

where $I\left(\xi,\eta\right)$ is the intensity of a typical source point, $K\left(\xi,\eta; x_{\mathrm{det}}, y_{\mathrm{det}}\right)$ is the transmission function of the optical scheme describing the radiation propagation from this point to a given point in the detector plane. In the case of an in-line scheme – source-object-detector – $K\left(\xi,\eta; x_{\mathrm{det}}, y_{\mathrm{det}}\right)$ is simply the Kirchhoff–Fresnel integral and expression (1) takes the form

$$I\left(x_{\mathrm{det}}, y_{\mathrm{det}}\right) = \int_{\sigma} I\left(\xi,\eta\right)\left|\int_{S} t\left(x_o, y_o\right)\frac{e^{ik\left(r_{so}+r_{od}\right)}}{r_{so}r_{od}}\Lambda dx_o dy_o\right|^2 d\xi d\eta \tag{2}$$

where x_o, y_o are the coordinates in the object plane S, r_{so} and r_{od} are the distances between the source – object and object – detector, respectively, σ is the source plane and Λ is an inclination factor which is equal to $\Lambda = (i/2\lambda)\left(\cos(\vec{n}, \vec{r}_{so}) - \cos(\vec{n}, \vec{r}_{od})\right) \cong i/\lambda$ in the paraxial approximation, $t\left(x_o, y_o\right)$ is the object transmission function, $\vec{n}$ is the vector of external normal, $k = 2\pi/\lambda$ is the wave number (wave vector modulus), and λ is the X-ray wavelength. For the paraxial approximation the following expressions are valid

$$\Lambda \cong i/\lambda; \qquad r_{so} \cong R_1 + \frac{\left(x_o-\xi\right)^2}{2R_1} + \frac{\left(y_o-\eta\right)^2}{2R_1};$$

$$r_{od} \cong R_2 + \frac{\left(x_o-x_{\mathrm{det}}\right)^2}{2R_2} + \frac{\left(y_o-y_{\mathrm{det}}\right)^2}{2R_2}$$

$$I\left(x_{\mathrm{det}}, y_{\mathrm{det}}\right) = \int_{\sigma}\left|e^{ik(R_1+R_2)}\underbrace{\int_{S}\frac{\sqrt{|I\left(\xi,\eta\right)|}}{R_1}e^{i\frac{k}{2R_1}\left[\left(x_o-\xi\right)^2+\left(y_o-\eta\right)^2\right]}t\left(x_o, y_o\right)}_{\downarrow\; U^{in}(x_o,y_o)}\right.$$

* Corresponding author at: Institute of Microelectronics Technology and High Purity Materials, Russian Academy of Sciences, Chernogolovka, Moscow Region, Chernogolovka, Academician Ossipyan str, 6, 142432, Russia.
E-mail address: igor@iptm.ru (I.A. Schelokov).

https://doi.org/10.1016/j.optcom.2017.09.070
Received 17 July 2017; Received in revised form 19 September 2017; Accepted 21 September 2017
0030-4018/

$$\times \frac{e^{i\frac{k}{2R_2}\left[(x_o-x_{\mathrm{det}})^2+(y_o-y_{\mathrm{det}})^2\right]}}{R_2}\Lambda dx_o dy_o\Bigg|^2 d\xi d\eta \tag{3}$$

where R_1 and R_2 are the distances between the source – object and object – detector planes along the optical axis, respectively.

In the expression above the part describing the field amplitude distribution in the incident radiation clearly stands out. It is this part that allows the development of an algorithm to describe the transition from plane to plane in a multicomponent system.

A direct or standard scheme of simulation or calculation of expressions (1)–(3) includes

- a radiation source presented as an array of point sources
- wave-field distributions successively calculated in all planes for each source point
- the resulting pattern is obtained by incoherent summation of the contributions from all source points with a weighting factor equal to the source intensity for a given point, i.e. the *intensities* of calculated diffracted fields *are summed*.

The most significant point in such an approach is the step of spatial sampling on which basis the expressions are calculated. It is this step that determines the computational burden for a stated problem. The amount of time taken is determined by the precision of calculating the Fresnel type integral convolutions. Explicitly, this dependence is expressed in terms of the size of the last Fresnel zone Δr_n, where n is the number of Fresnel zones per the beam aperture A (see Discussion in [2]). The number of partition points N should then be larger than

$$N \geq \frac{A}{\Delta r_n} = \frac{A^2}{F\lambda} \tag{4}$$

so that no less than one point be per each sign-alternating (according to the contribution to the integrand) Fresnel zones, where $1/F = 1/R_1 + 1/R_2$. Thus, the number of partition points increases with the square of the beam aperture and is inversely proportional to the X-ray wavelength. For example, the necessary number of partition points to consider the problem of a 0.4 mm wide beam transition through the optical scheme (F = 5 cm, λ = 1.54 Å) is 2^{16}–2^{18} per the beam cross section for each image coordinate.

Expression (4) might suggest, at the first sight, that the sampling step is determined by the precision of convolution integral calculation and does not depend on the spatial resolution δ of an optical scheme ($\delta = \xi_s \cdot R_2/R_1$, where ξ_s is the source size). In fact, this is not quite correct. Let consider what really occurs in some detail.

When we represent a source as an array of point sources and study an optical system response to its illumination with each of the point sources, this means that we study an optical system under the condition of diffraction limit of spatial resolution. This study requires a very fine sampling with a maximally permissible step equal to the last Fresnel zone size in the beam aperture. When averaged to the source by incoherent summation of contributions of point sources resulting from the partition, the spatial resolution is specially deteriorated to a required value. To put it otherwise, to obtain a required result we seem to intentionally deteriorate the resolution. In fact, within this approach the spatial sampling is chosen such as if the stated problem is to be solved for an optical system with the diffraction limit by resolution. As a result, computational resources would suffice only to simulate small-aperture schemes or small parts of a general scheme.

An alternative approach exists to describe optical systems. It is based on the second-order correlation function termed mutual intensity. Its basis is the Van Cittert–Zernike theorem which allows the calculation of the mutual intensity of an incoherent source and the theorem of mutual intensity propagation. Transform (2) to (Fig. 1)

$$\begin{aligned} I\left(x_{\mathrm{det}}, y_{\mathrm{det}}\right) &= \int_\sigma I\left(\xi,\eta\right)\left(\int_S t\left(x_o, y_o\right)\frac{e^{ik(r_{so}+r_{od})}}{r_{so}r_{od}}\Lambda dx_o dy_o\right) \\ &\times\left(\int_S t\left(x_o, y_o\right)\frac{e^{ik(r_{so}+r_{od})}}{r_{so}r_{od}}\Lambda dx_o dy_o\right)^* d\xi d\eta = \\ &= \int_\sigma I\left(\xi,\eta\right)\iint_S t\left(x_{o1}, y_{o1}\right) t^*\left(x_{o2}, y_{o2}\right)\frac{e^{ik(r_{so1}-r_{so2})}}{r_{so1}r_{so2}} \\ &\times\frac{e^{ik(r_{od1}-r_{od2})}}{r_{od1}r_{od2}}\Lambda_1\Lambda_2^* dx_{o1}dy_{o1}dx_{o2}dy_{o2}d\xi d\eta = \\ &= \iint_S \underbrace{\int_\sigma I\left(\xi,\eta\right)\frac{e^{ik(r_{so1}-r_{so2})}}{r_{so1}r_{so2}}d\xi d\eta}_{J\left(x_{o1},y_{o1};x_{o2},y_{o2}\right)\leftarrow\text{mutual intensity}} t\left(x_{o1}, y_{o1}\right) t^*\left(x_{o2}, y_{o2}\right) \\ &\times\frac{e^{ik(r_{od1}-r_{od2})}}{r_{od1}r_{od2}}\Lambda_1\Lambda_2^* dx_{o1}dy_{o1}dx_{o2}dy_{o2} \end{aligned} \tag{5}$$

In the above expression, use is made of the fact that the product of two integrals (or two infinite sums) gives a double integral on the surface of an object S, where the points (x_{o1}, y_{o1}) and (x_{o2}, y_{o2}) take on independently all positions on the surface S of integration. Rewriting the expression for the function of mutual intensity in the paraxial approximation gives the Van Cittert–Zernike theorem which was just proved above. The inclusion of extra dimensionalities into the expressions makes them cumbersome, therefore the formulae in the text below will be given for a one-dimensional case. Generalization to the 2D case is possible although not quite trivial. So, in the paraxial approximation the 1D case is

$$\Lambda \cong i/\lambda; \qquad r_{so(1,2)} \cong R_1 + \frac{\left(x_{o(1,2)} - \xi\right)^2}{2R_1}$$

$$\begin{aligned} J_{in}\left(x_{o1}, x_{o2}\right) &= \int_\sigma I\left(\xi\right)\frac{e^{i\frac{k}{2R_1}\left\{(x_{o1}-\xi)^2+\left((x_{o2}-\xi)^2\right)\right\}}}{R_1}d\xi \\ &= \int_\sigma \frac{I\left(\xi\right)}{R_1}e^{i\frac{k}{2R_1}\left\{x_{o1}^2-x_{o2}^2-2\xi(x_{o1}-x_{o2})\right\}}d\xi \\ &= \frac{e^{i\frac{k}{2R_1}\left\{x_{o1}^2-x_{o2}^2\right\}}}{R_1}\widetilde{I}\left(-\frac{\left(x_{o1}-x_{o2}\right)}{\lambda R_1}\right) \end{aligned} \tag{6}$$

where $\widetilde{I}$ denotes the Fourier transform of $I\left(\xi\right)$ and J_{in} is incoming mutual intensity from the source.

The theorem of mutual intensity propagation for an in-line set-up in the paraxial approximation for the one-dimensional case states

$$\begin{aligned} &J_{out}\left(x_{o1}, x_{o2}\right) = J_{in}\left(x_{o1}, x_{o2}\right) t\left(x_{o1}\right) t^*\left(x_{o2}\right) \\ &J\left(x_{d1}, x_{d2}\right) = \int_S J_{out}\left(x_{o1}, x_{o2}\right)\frac{e^{i\frac{\pi}{\lambda R_2}\left\{(x_{o1}-x_{d1})^2-(x_{o2}-x_{d2})^2\right\}}}{\lambda R_2}dx_{o1}dx_{o2} \\ &I\left(x_{\mathrm{det}}\right) = J\left(x_{d1} = x_{d2} = x_{\mathrm{det}}\right) \end{aligned} \tag{7}$$

here J_{out} denotes the outcoming mutual intensity from the object plane and J and I are the mutual intensity and the intensity in the detector plane, respectively.

This approach is widely used in theoretical analysis of optical systems [1,3,4] although its application to problems of optical simulation is scarce. Even though the Fourier transformation substitutes for the point-by-point partition of the source in the expressions, its "cost" is addition of an extra dimensionality and, correspondingly, substitution of a two-dimensional convolution by a four-dimensional with all the drawbacks of the 2D one (i.e. squared growth of the number of partition points, depending on the beam aperture for each integration variable). This cost is too high. Nevertheless it is worth mentioning that this approach supposes integration over the source at the very first step of computation. In the 3rd Section of this paper we show the advantages of this approach. Summing up, the Table 1 for comparison can be proposed.