Holographic and diffractive x-ray imaging using waveguides as quasi-point sources

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Abstract. We report on lensless nanoscale imaging using x-ray waveguides as ultra-small sources for quasi-point-like illumination. We first give a brief account of the basic optical setup, an overview of the progress in waveguide fabrication and characterization, as well as the basics of image formation. We then compare one-step holographic and iterative ptychographic reconstruction, both for simulated and experimental data collected on samples illuminated by waveguided beams. We demonstrate that scanning the sample with partial overlap can substantially improve reconstruction quality in holographic imaging, and that divergent beams make efficient use of the limited dynamic range of current detectors, regardless of the reconstruction scheme. Among different experimental settings presented, smallest source dimensions of 29 nm (horizontal) × 17 nm have been achieved, using multi-modal interference effects. These values have been determined by ptychographic reconstruction of a Ta test structure at 17.5 keV and have been corroborated by simulations of field propagation inside the waveguide.

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1. Introduction

Lensless coherent x-ray imaging offers a unique potential to image functional assemblies in four dimensions at the nanoscale, with promising applications both in material and life sciences. The lensless approach is developed to overcome the limits imposed by fabrication technology of diffractive and refractive x-ray lenses [1, 2]. Although optical elements, such as focusing mirrors, compound refractive lenses, Fresnel zone plates, capillaries or waveguides, may still remain important components of the optical system, the image resolution should not be determined by the precision with which these components can be fabricated. In the conceptually simplest version of coherent diffractive imaging (CDI), the far field diffraction pattern of a sample illuminated with a (nearly) flat wave front is measured and used as an input for iterative reconstruction [3]–[7]. The primary data input is thus the intensity of the scattered wave. Phase information is retrieved from the accurately sampled coherent diffraction pattern by using additional constraints in real space (a priori information), such as finite support, positivity or overlap constraints when the sample is shifted. An alternative and possibly complementary approach to solve the phase problem associated with lensless imaging is holographic phase retrieval, making use of the interference terms between a scattered and a reference wave to encode phase information [8], possibly with less restrictive a priori information. By interference with a strong reference wave, a weak scattering amplitude can be amplified high above background signals of residual scatter. To implement this holographic scheme at the nanoscale, quasi-spherical reference waves can be used to yield a magnified hologram of the sample, combining the ideas of Fresnel (holographic) imaging and x-ray projection magnification [9]. Such holographic x-ray projection experiments have shown to yield quantitative images of hard and soft materials in electron density contrast [10], magnetization contrast [11] or specific elemental contrast [12]. An extension from two-dimensional (2D) projection images to three-dimensional (3D) data sets by holographic tomography is relatively straightforward [13]. In contrast to iterative image reconstruction by CDI algorithms [14], where central issues of uniqueness, convergence, reconstruction speed, as well as optimum choice of initial
phases are yet unsolved in a strict mathematical sense, holographic reconstruction is a one-step deterministic reconstruction process. Combinations of holographic and iterative phasing therefore seem to be a particularly promising route [15].

To generate reference waves for holography, pinholes can be used, either in the in-line [12], off-axis or Fourier holography [11] setup. Small pinholes in absorbing metal foils down to diameters in the range of a few hundred nanometers can be fabricated for example by focused ion beam techniques. However, to increase resolution, smaller and smaller aperture diameters lead to an inversion of the thickness/diameter aspect ratio, and the propagation can no longer be described by 2D absorption masks, but must be treated by 3D field propagation in stratified media with a distinct mode structure that can be used to the advantage of coherence filtering. The corresponding transition from a pinhole to a waveguide has been studied in detail before [16].

To increase the intensity of the reference beam, a focused beam is coupled into the waveguide front side. X-ray waveguides (WG) can thus be used as ultra-small quasi-point sources to filter and to deliver x-rays at nanoscale dimensions, replacing the function of macroscopic slits and pinholes of conventional x-ray experiments. In the mono-modal regime they enable control of the wave front phase highly desirable for coherent x-ray imaging and holography [10, 17]. Depending on the materials employed for the guiding and cladding layers, waveguides can be used to shape beams with cross-sections down to about 10 nm [18], below the values currently achieved by focusing optics [1, 2, 19]. Furthermore, the coherence properties and cross-section of the beam are decoupled from the primary source. Finally, over-illumination and stray radiation, often accompanying other forms of x-ray focusing (with far field optics), are efficiently blocked by the cladding and cap layers.

In this paper, we report on recent progress in waveguide-based x-ray imaging, with special emphasis on design and fabrication of waveguides, image formation and reconstructions. While our aim is to develop this scheme for imaging of biological cells and tissues, we concentrate here on preparatory work and give examples based on simulated imaging experiments on biological samples and suitable test patterns with well-controlled structure size and contrast. Finally, reconstructions from experimental data of such a test structure will be presented and discussed. The basic experimental setup for waveguide-based holographic microscopy of test objects and biological cells, as discussed in the following sections, is presented in the form of an overview schematic in figure 1. The monochromatic synchrotron beam is focused by a high-gain Kirkpatrick–Baez (KB) mirror optics [20] into a 2D waveguide channel with a guiding core of a diameter in the range of 10–100 nm. Note that KB focusing and x-ray waveguide optics are both essentially non-dispersive, so that broad bandpass (pink beam) experiments become possible. The exiting divergent wave field may correspond to a superposition of the supported waveguide modes or, in the case of single-mode waveguides, to a fully coherent single mode. After illumination of the sample, a magnified in-line hologram of the sample is recorded on a CCD or single-photon counting detector. Freeze-dried cells attached on a thin polyimide (Kapton) film are positioned and monitored in the x-ray beam by an in situ optical microscope with a hole drilled through the objective to allow for the passage of the x-ray beam.

To study the feasibility of waveguide-based imaging on unstained biological samples at multi-keV photon energies, an experiment was simulated with relevant parameters. The reconstruction of the simulated hologram reproduces the cell phantom used in the simulation down to very fine structures. Note that biomolecular samples in a multi-keV x-ray beam act in most cases as pure, but not always weak phase objects. For the simulation, the maximum phase shift and amplitude attenuation of a 3 µm thick biological cell with 66% protein content
Figure 1. (a) Schematic of the experimental setup used for waveguide-based holographic microscopy of test objects and biological cells. Illumination of the sample by the divergent waveguide beam yields a magnified in-line hologram on the detector. For illustration, freeze-dried cells attached on a thin polyimide (Kapton) film are shown, which can be positioned in the x-ray beam and monitored by an in situ optical microscope with a hole drilled through the objective to allow the passage of the x-ray beam. The reconstruction of the simulated hologram shows the cell phantom used in the simulations. (b) Geometry of the imaging experiment with the waveguide idealized as a point source illuminating the sample. (c) Equivalent plane wave geometry (see section 4.3) with an effective sample–detector distance of $z = z_1/z_2/(z_1 + z_2)$ and a detector pixel size demagnified by a factor $M = z_2/z_1$. The one-to-one correspondence is only given within the small-angle approximation which is, however, always valid in view of typical waveguide divergence on the order of 1 mrad.

and a 6 nm thick outer lipid layer, illuminated at 17.5 keV photon energy, were estimated as $\Delta \phi = 0.174$ rad and $A = 1.16 \times 10^{-4}$, respectively. The stoichiometry of the protein and lipid content of the cell was used as suggested in [21]. The hologram was simulated based on a total flux of $1 \times 10^7$ photons, assuming Poissonian shot noise. The waveguide exit wave was assumed as a Gaussian function with a full-width at half-maximum of the intensity of 20 nm in the waveguide exit plane. The waveguide exit plane was located 1.1 mm upstream of the sample, which in turn was assumed to be 3 m away from the detection plane. The reconstruction was

obtained from the hologram by a single numerical operation (free space back-propagation). The resulting reconstructed phase image of the cell phantom indicates that holographic imaging of unstained biological objects in a multi-keV beam should be possible up to a very high phase sensitivity.

The schematics in figures 1(b) and (c) illustrate the basic concept of cone beam and parallel beam in-line holography, where the scattered wave of a point scatterer is superimposed with the parallel and divergent reference (primary) beam, respectively.

The paper is organized as follows: after this introduction, a brief overview about the fundamentals of x-ray waveguide optics is presented in section 2, before addressing recent progress in fabrication of waveguides in section 3. Image formation and holographic reconstruction are addressed in section 4, followed by illustrative simulations, including a holographic and also an iterative reconstruction (section 5). Recent experimental results are given in section 6, before the paper closes with a brief outlook.

2. Waveguide optics: a brief overview

A few analytical solutions for x-ray waveguide mode propagation are known for simple paradigmatic examples and are derived from the corresponding treatment of guided waves well established in other fields such as optical waveguides [22]. The examples serve as an instructive basis for the more general problem, treated by simulations. Parameters, approximations and coupling geometries specific to x-ray waveguides have been presented in [23]–[26]. For a brief overview, we consider a scalar wave function \( \Psi(x, y, z) \), where \( \Psi \) could, for example, denote the electric field of a \( y \)-polarized beam propagating in the \( z \)-direction within a layered structure characterized by an index profile (or scattering potential) with piecewise constant refractive index \( n_j(x) = 1 - \delta_j + i\beta_j \) for the \( j \)th layer. Starting from the Helmholtz equation

\[
\Delta \Psi + k_0^2 n^2(x) \Psi = 0,
\]

where \( k_0 = 2\pi/\lambda \) is the vacuum wave vector, the ansatz \( \Psi(x, y, z) = \psi(x)\exp(i\xi z) \) with the so-called propagation constant \( \xi \), leads to the ordinary differential equation

\[
\psi''(x) + \left(k_0^2 n^2(x) - \xi^2\right)\psi(x) = 0.
\]

Away from absorption edges, the phase shifting contribution of the refractive index is described by \( \delta(x) = 2\pi r_0 \rho(x)/k_0^2 \), with \( r_0 \) denoting Thomson’s scattering length or the classical electron radius, and \( \rho(x) \) the electron density. \( \delta \) thus depends on the photon energy and on the material, with typical values on the order of \( 10^{-6} \) for hard x-rays. The absorption coefficient \( \beta \) is typically two orders of magnitude smaller and can be neglected for the determination of modes. Omitting the \( \delta^2 \)-terms in \( n^2 \), the Helmholtz equation can be rewritten in the form

\[
\psi''(x) - 2\delta(x)k_0^2 \psi(x) = (\xi^2 - k_0^2)\psi(x) =: \Lambda \psi(x),
\]

representing an eigenvalue problem with the mode eigenvalue \( \Lambda \), and with the boundary conditions appropriate for the resonant beam or front-coupling regime.

For simple waveguide geometries, e.g. a planar waveguide with a single guiding layer of width \( d \) with refractive index \( n_1 \) in a cladding with index \( n_2 \) and a propagation constant \( n_2^2k_0^2 < \xi^2 \) (bound modes), a solution of equation (2) can be written as

\[
\Psi(x) = \begin{cases}
Ae^{\gamma x} & \text{for } -\infty < x < 0, \\
A \cos(\kappa x) + B \sin(\kappa x) & \text{for } 0 \leq x \leq d, \\
C e^{-\gamma (x-d)} & \text{for } d < x < +\infty,
\end{cases}
\]

with \( \kappa = \sqrt{k_0^2n_1^2 - \zeta^2} \) and \( \gamma = \sqrt{(n_1^2 - n_2^2)k_0^2 - \kappa^2} \). The latter condition along with the transcendental eigenvalue equation \( \tan(\kappa d) = 2\kappa \gamma / (\kappa^2 - \gamma^2) \) determines the modes. Solving the transcendental equation, one obtains a fixed number \( N \) of resonant modes at parameters \( \kappa_N \), where \( N \) only depends on \( \rho_1, \rho_2 \) and \( d \). An important limiting case is the critical (maximum) guiding layer width \( W_c = \pi / k_0 \sqrt{2\delta} \) of a waveguide with ideal interfaces and vacuum guiding layer, at and below which the waveguide supports only a single mode, forming a fundamental length scale of x-ray waveguide optics. At the same time, it fixes the waveguide width \( d_{min} \) of the highest possible wave confinement, e.g. for rectangular waveguides \( d_{min} = W_c / \pi [18, 27] \). The intensity distribution of the wave broadens both for larger and smaller \( d_{min} \), since the evanescent waves in the cladding become more pronounced, if \( d \) is reduced below \( W_c \).

We now turn from this simple one-dimensional WG (1DWG) geometry to the 2D analogue of a rectangular WG with

\[
n(x, y) = \begin{cases} n_1 & \text{for } 0 \leq x \leq d_x \text{ and } 0 \leq y \leq d_y, \\
n_2 & \text{else},
\end{cases}
\]

(4)

where \( d_x \) and \( d_y \) denote the guiding core width and height, respectively. The 2D-Helmholtz equation,

\[
\frac{\partial^2 \psi(y, x)}{\partial y^2} + \frac{\partial^2 \psi(y, x)}{\partial x^2} + (n(y, x)^2k^2 - \zeta^2)\psi(y, x) = 0,
\]

(5)

cannot be solved analytically any more. Only by neglecting the corner regions, an analytical approximation becomes possible which is formed by factorization of the independent solutions corresponding to two orthogonal one-dimensionally confining waveguides. For more general geometries of 1D and 2D waveguides (1DWGs and 2DWGs, respectively), x-ray propagation in waveguide channels must be studied by finite difference (FD) simulations [16], [28]–[30], capable of describing also more complex structures and effects including both thickness variations and roughness [27, 31]. These field simulations are based on the parabolic (paraxial) approximation, which is valid if the local wave vector of the propagating beam is coaxial with the propagation direction \( z \) within an angular range of the order of the critical angle.

Figure 2 shows the wave propagation in a 2DWG structure as simulated by FD calculations. Parameters were chosen as used for the imaging experiment described below, i.e. the void waveguide channel with a length of \( \ell = 13 \) mm along the optical axis and lateral dimensions of \( 140 \) nm (hor.) \( \times 24 \) nm (vert.) was assumed to be embedded in Si and illuminated at a photon energy of \( E = 17.5 \) keV. The field distributions in horizontal and vertical directions were regarded as factorizable and therefore calculated independently in the geometry of a 1DWG.

While in the vertical direction only a single mode is formed with a full-width at half-maximum (FWHM) intensity of about 19 nm, the wider horizontal opening of the waveguide supports multiple modes varying in width from 20 nm (second order) to 34 nm (zeroth order). The final lateral width of the exit wave is difficult to predict from field simulations inside the guiding channel and may depend on the ratio of the WG length \( \ell \) and the period length of the field along the optical axis, the roughness of the inner channel walls as well as the coupling of the pre-focused beam into the waveguide. However, these idealized simulations indicate that the wave exiting a multiple mode waveguide very likely has a substantially smaller lateral extension than the respective geometrical width of the waveguide channel.
Figure 2. Field simulations of the parabolic wave equation by finite difference (FD) equations. The waveguide was modeled as a vacuum channel with dimensions 140 nm (hor.) × 24 nm (vert.) × 13 mm (axial), embedded in Si and illuminated with a photon energy of $E = 17.5$ keV. Simulated vertical and horizontal intensity distributions along the optical axis are shown in (a) and (b), respectively, normalized to the intensity directly in front of the waveguide. Magnified regions of interest (subfigures (c) and (d)) clearly show the single (c) and multiple (d) mode structures inside the guiding core. Profiles of the multiple mode distribution along the horizontal axis perpendicular to the direction of the beam illustrate the different possible lateral dimensions of the field distribution in a multiple mode waveguide (e).

3. Fabrication of second-generation x-ray waveguides

While planar 1DWGs are relatively easy to fabricate, and have been given much attention in the literature, they are of relatively limited use for holographic imaging, for which 2DWGs as quasi-point sources are needed. The main challenge consists in fabrication of two-dimensionally confining waveguides with suitable specifications. A first successful effort toward 2DWGs was presented in [25], with however impractically low flux, associated with the coupling geometry (resonant beam coupling). The first successful 2DWG-based holography experiments were achieved in [10, 32], in the front-coupling regime, where the pre-focused synchrotron beam impinges normal to the waveguide entrance plane, rather than under grazing incidence through a thinned cladding as in resonant beam coupling devices. For both coupling geometries, the so-called first-generation 2DWG channels consisted of polymer stripes defined by e-beam lithography coated with a metal or silicon cladding [25, 26]. Optical properties, particularly the
transmission and mode structure, were still severely limited by fabrication and real structure effects. While ideal waveguide channels should be empty (filled with air), a polymer filler material can lead to unnecessary absorption, unwanted phase front modulations based on density variations, as well as drift resulting from beam damage.

To overcome these problems, we have started two alternative and complementary approaches to second-generation 2DWGs, see figure 3. The first approach illustrated in the upper row of figure 3 yields empty (air) channels in silicon wafers covered by wafer bonding (bonded-2DWGs), and can be adapted in length to match the requirements of a wide range of photon energies. For fabrication of bonded-2DWGs, channels are etched into silicon wafers using an etch mask defined by e-beam lithography. After removal of the mask, a second wafer is bonded on top of the first as a capping layer. The principal ideas of this scheme are presented in [33, 34], where however only µm sized cross-sections were achieved in the horizontal direction. Further
refinement of the method has yielded bonded-2DWGs in the relevant sub-100 nm range (see figure 3).

The second approach, illustrated in the lower row of the figure, is based on crossed 1DWG slices (crossed-2DWG), each slice with a thickness in the range $\ell = 0.1–3$ mm. The slices consist of stable sputtered thin films, with amorphous C as the guiding layer. By generalizing the index profile to a two-component cladding, transmission can be optimized [35], even for very small $d$. Waveguiding in 1DWG slices as small as $d \leq 10$ nm has been demonstrated in the meantime. By combination of two high transmission 1DWG slices glued onto each other in a crossed geometry, an effective 2D quasi-point source for holographic imaging can be formed. Compared to the previous serial arrangement of two crossed 1DWGs [36], the setup is much more compact, so that the horizontal and vertical focal planes coincide. The design and choice of materials, and in particular of Ge as a cladding material allow for a small total waveguide length $\ell < 500$ $\mu$m, but currently limit the applications to higher photon energies $E \geq 12$ keV.

Fabrication starts with a layer sequence of planar optical films. For matter of concreteness, we give the values of the first recent realization of a crossed-2DWG: the layer sequence Ge/Mo[$d = 30$ nm]/C[$d = 35$ nm]/Mo[$d = 30$ nm]/Ge, deposited by magnetron sputtering on 3 mm thick Ge single crystal substrates (Incoatec GmbH, Germany). The interlayer thickness of $d_i = 30$ nm is designed to encompass the evanescent wave components of the propagating mode. The profile of the index of refraction $n = 1 - \delta + i\beta$ in the two-component waveguide is optimized for high transmission [35]. The idea can best be illustrated by examination of the dispersion $\delta$ and absorption $\beta$ coefficients for a given experimental photon energy, e.g. $E = 17.5$ keV. The C layer embedded in the high $\delta_{Mo} = 1.49 \times 10^{-6}$ Mo cladding forms a relatively deep potential well. At the same time, a relatively low $\beta_{Mo} = 1.01 \times 10^{-7}$ value of Mo reduces the absorption in the (interlayer) cladding and hence enables an increased transmission. Note that at this energy, the low electron density C layer with $\beta_{C} = 2.77 \times 10^{-10}$ contributes less than 2% to the effective absorption $\mu_{eff}$. In other words, C ‘acts’ essentially like a vacuum guiding layer.

Before dicing and arrangement of the crossed slices, the optical films have to be capped. A sputtered Ge layer of 1 $\mu$m thickness serves as a first capping and protection layer, onto which a second Ge layer is fixed by an alloying process to block the beam components not impinging onto the waveguide entrance. The waveguide slice is then cut by a diamond wafer dicer to the desired thickness. For example, thicknesses of 400 and 207 $\mu$m have been used for the horizontal and vertical components of a crossed-2DWG operated at 17.5 keV. For cleanup of the front end exit surfaces, the slices can be treated using focused ion beam (FIB) polishing. Figure 3(e) shows the polished entrance area of the 1DWG slice with the smallest guiding layer achieved so far ($d = 9$ nm).

4. Theory of holographic image formation and reconstruction

The image formation of holographic (projection) microscopy based on a hard x-ray quasi-point source can be described by free space propagation after modulation of the spherical wave front by the object [17], [37]–[39]. With increasing resolution and photon energy needed to penetrate bulk samples, absorption contrast becomes negligible and phase contrast prevails. We first consider the interaction of the beam with the sample in the so-called projection approximation. We then discuss image formation via propagation (direct problem), and finally the process of object reconstruction, based on simple holographic single-step back-propagation. The process

of image formation and reconstruction from the observed intensity pattern is illustrated by numerical simulations in section 5 and forms the bases for the following experiments section 6. For comparison, more elaborate iterative reconstructions are also applied, both for simulated and experimental data.

4.1. Interaction of a coherent beam with a thin sample

We consider an optically ‘thin’ sample located in the object plane and illuminated by a plane wave $\psi_{in}$. For a ‘thin’ object, the (complex-valued) optical transmission function $\tau(x, y)$ relating the exit to the incident wave $\psi_{out}(x, y) = \tau(x, y) \times \psi_{in}$ is simply given by the projection of the local index of refraction $n(x, y, z) = 1 - \delta(x, y, z) + i\beta(x, y, z)$ over the sample thickness $t$ along the direction of propagation parallel to the z-axis. The real and imaginary components of the index determine the phase shift $\phi(x, y)$ and the attenuation $\mu(x, y)$, respectively,

$$
\tau(x, y) = \exp \left[ ik \left( 1 - \int_0^t n(x, y, z) \, dz \right) \right]
$$

$$
= \exp [ikt] \exp [i\phi(x, y) - \mu(x, y)/2].
$$

For simplicity the index 0 of the vacuum wavenumber $k = 2\pi/\lambda$ has been suppressed. For samples that are uniform in $z$, and if resonant effects close to absorption edges can be neglected, $\phi = -k\delta t \approx \rho_e r_0 t \lambda$ and $\mu = 2k\beta t$. For inhomogeneous, but non-absorbing samples the phase shift is simply proportional to the projected electron density of the material. For the validity of equation (7) we refer to the general literature on the first Born approximation and to [40, 41] in particular, which give the criterion $D|\Delta n| < 2\pi \lambda C \approx \pi \lambda$, with the sample thickness $D$, the refraction index contrast $|\Delta n|$, and $C \leq 1$ a constant.

4.2. Contrast formation by propagation

Following [38, 42] we discuss propagation imaging in the limit of a weak phase object. For studies of thin slices and single cells, the weak phase object approximation discussed below is very well justified [43].

The wave field $\psi_2(x_2, y_2)$ in the detector plane $S_2$, downstream from the object plane $S_1$, is determined by a linear superposition of waves $\psi_1(x_1, y_1)$ exiting from the object plane. After transformation to Fourier space (indicated by a tilde), this propagation reduces to a simple multiplication $\tilde{\psi}_2 = \tilde{h}_z \times \tilde{\psi}_1$ with the free space propagator [44]

$$
\tilde{h}_z = \exp \left( ikz\sqrt{1 - \lambda^2 v_x^2 - \lambda^2 v_y^2} \right),
$$

with spatial frequencies $v_x$ and $v_y$. If the paraxial approximation is valid, i.e. if $k \gg 2\pi v_{x,y}$ [44], $\tilde{h}_z$ can be simplified to the propagator $\tilde{h}_z^{(F)} := \exp \left[ ikz \left( (1 - \lambda^2 v_x^2 + \lambda^2 v_y^2)/2 \right) \right]$ describing paraxial (Fresnel) propagation.

If the sample with complex transmission $\tau(x, y)$ is illuminated by a plane wave $\psi_{in}$, the paraxially propagated field in plane $S_2$ is thus given as

$$
\tilde{\psi}_2(v_x, v_y) \simeq \left[ \delta_D(v_x, v_y) + i\phi(v_x, v_y) - \tilde{\mu}(v_x, v_y)/2 \right] \exp \left[ ikz - i\pi \lambda z(v_x^2 + v_y^2) \right],
$$
where \( \delta_D \) denotes the Dirac delta function representing the directly transmitted beam. To first order in \( \phi \) and \( \mu \) (weak object approximation) the corresponding intensity \( \bar{I} = |\bar{\psi}_2|^2 \) is given in Fourier space by [38]

\[
\bar{I}(\nu_x, \nu_y) \approx \delta_D(\nu_x, \nu_y) + 2\phi(\nu_x, \nu_y) \sin \chi - \mu(\nu_x, \nu_y) \cos \chi
\]

(10)

with \( \chi = \pi \lambda z(\nu_x^2 + \nu_y^2) \). \( \sin \chi \) and \( \cos \chi \) in this equation are termed the phase and amplitude contrast transfer functions (CTFs). The oscillatory behaviour with respect to the spatial frequencies of the object and the distance between object and detector is the characteristic feature of free space propagation, and has been validated experimentally for the relevant sample and beam parameters [43].

4.3. Holographic and iterative reconstruction in waveguide-based imaging

Above we have considered the propagation of a field \( \psi_{\text{out}} = \tau \times \psi_{\text{in}} \) behind a sample illuminated by a plane wave \( \psi_{\text{in}} \). Obviously, with waveguides as point-like sources this parallel-beam geometry has to be modified to account for the divergence of the waveguide field illuminating the sample.

For the following discussion of the image formation and holographic reconstruction process we consider a propagation setup with three planes, as illustrated in figure 1: waveguide exit plane \( S_0 \), sample plane \( S_1 \) at a distance \( z_1 \) from \( S_0 \), and finally the detector plane \( S_2 \) at a distance \( z_2 \gg z_1 \) downstream of \( S_1 \). The illumination field \( \psi_{\text{ill}}^1 = h_1[\psi_0] \) is the propagated field of a waveguide emitter incident on the sample, where \( h_1 \) denotes the real space version of the free space propagator (for a definition of the defocus distance \( z \), see below or the caption of figure 1). \( \psi_0 \) is the waveguide exit field, and \( \psi_1 = \tau \times \psi_{\text{ill}}^1 \) the sample exit wave. Finally, the field in the detector plane is given as \( \psi_2 = \mathcal{F}[\psi_1] \) with intensity \( I \propto |\psi_2|^2 \). Here \( \mathcal{F}[\ldots] \) denotes the Fourier transform operation. For all practical situations in holographic projection the detector is in the Fraunhofer regime with respect to diffraction from the sample plane. If in turn the Fresnel number describing the propagation from the WG to the sample, i.e. \( F = d^2/(\lambda z_1) \ll 1 \), which is generally also the case here, the sample is illuminated by a quasi-spherical wave of the form [45]

\[
\psi_{\text{ill}}^1(x_1, y_1) \approx \frac{\exp(ikz_1)}{i\lambda z_1} \left( \int_{\text{field of a point source}} \psi_0(x_0, y_0) \exp \left( \frac{ik(x_1 x_0 + y_1 y_0)}{z_1} \right) \ dx_0 \ dy_0 \right) \]

(11)

As \( \psi_0 \) obeys an inversion symmetry, the empty waveguide far field amplitude is a real quantity, so that the reference wave in the sample plane can be described as a spherical wave enveloped by the waveguide far field amplitude.

Considering a typical waveguide divergence on the order of 10^{-3} rad the paraxial approximation is still valid for the propagation between waveguide and the sample. Importantly, it has been shown [38, 45] that within this approximation the projection geometry of a divergent beam emitted from a point source can be mapped onto the parallel beam geometry considered in section 4.2. Given a distance \( z_1 \) between source and sample and \( z_2 \) between sample and detector, the paraxial illumination of the sample by a point source can be described by a plane-wave illumination of the sample and subsequent free space propagation of the exit wave over an effective propagation (defocus) distance \( z = z_1 z_2/(z_1 + z_2) \approx z_1 \) for \( z_2 \gg z_1 \). In this picture the hologram measured on the detector is demagnified by a factor \( M = (z_1 + z_2)/z_1 \approx z_2/z_1 \). After the coordinate transform from divergent to parallel propagation geometry, a simple plane
wave with the corresponding envelope can finally be used for holographic reconstruction by free space back-propagation.

4.4. Spatial resolution

Let us consider again the geometry sketched in figure 1. In the ray-optical model of a simple geometric projection from a small, but extended source the resolution is limited by the size of the source. However, this simple geometric picture breaks down as soon as the direct imaging regime ($\sin \chi \approx \chi$, see section 4.2) is left and the hologram more and more changes into a defocused far field image rather than a simple radiogram of the object. For the geometries considered here, typical values are $z_1 = 1\,\text{mm}$ and $z_2 = 3\,\text{m}$, so that for spatial periods $L < 1.5\,\mu\text{m}$ one obtains $\chi > 0.1$. Considering a typical waveguide divergence of $10^{-3}\,\text{rad}$ the illuminated spot on the sample is about $1\,\mu\text{m}$ in diameter, so that the image formation for all relevant spatial frequencies is essentially holographic and not radiographic.

Consequently, it seems appropriate to take up a more suitable diffraction-based point of view. Here the resolution is limited by the numerical aperture (NA) of the signal detected at the highest angle with respect to the optical axis and is thus given by $r_{\text{NA}} \approx \lambda/2\text{NA}$. Unless tails of the central waveguided cone or more generally scatter out of the central cone of radiation is used for reconstruction, the numerical aperture relevant for image formation is determined by the opening angle of the wave diffracted from the waveguide exit plane, i.e. the divergence of the waveguide beam. This in turn is given by the critical angle of total external reflection in the waveguide core, $\theta_c \approx \sqrt{2} \delta$. Thus the fundamental waveguide parameter introduced above, $W_c = \lambda/2\sqrt{2} \delta = \lambda/2\theta_c$, determines the resolution, at least in an order-of-magnitude sense. More generally, for a single-mode waveguide, i.e. for $d \lesssim W$, the resolution is roughly given by the waveguide diameter $d$

$$ r_{\Lambda_0} \approx d. \quad (12) $$

Here the index ‘$\Lambda_0$’ denotes the principal mode (order 0). Note that for multi-modal waveguides the resolution is generally not limited to the diameter of the waveguide, as superposition of modes can lead to sufficiently smaller exit wave sizes than the waveguide diameter (see above).

Another way to examine the waveguide divergence is given by idealizing the waveguide exit wave of a single-mode confining waveguide as a Gaussian beam, the well known solution to the paraxial wave equation. In the far field of a Gaussian beam amplitudes that have decayed by a factor of $1/e$ with respect to the central maximum are located on an axis pointing away from the optical axis by an angle of $\theta_{1/e} = \lambda/\left(\pi w_0\right)$, where $w_0$ is the $1/e$-decay radius at the beam waist in the waveguide exit plane [46]. The corresponding FWHM of the exit wave intensity is then given by $\Delta_{\text{FWHM}} = \sqrt{2 \ln 2} w_0$. Consequently, the half-angular $1/e$-divergence of the field amplitude is related to the FWHM value of the intensity at the WG exit plane via $\theta_{1/e} = \lambda/\sqrt{2 \ln 2}/(\pi \Delta_{\text{FWHM}})$. This in turn yields a resolution with respect to the $1/e$ decay of the field amplitude in the detector plane of $r \approx \lambda/(2\text{NA}) = \pi/(2\sqrt{2 \ln 2}) \Delta_{\text{FWHM}}$, i.e.

$$ r_{\text{Gauss}} \approx 1.33 \cdot \Delta_{\text{FWHM}}. \quad (13) $$

Here $\Delta_{\text{FWHM}}$ is the full width at half maximum of the intensity in the WG exit plane. It is well known that the FWHM of the intensity propagating in a single-mode waveguide is usually smaller than the waveguide diameter, i.e. $\Delta_{\text{FWHM}}/d \in [0.5, 1]$. In summary this result validates the use of a Gaussian beam as a model for the principal mode exiting a waveguide, as $r_{\Lambda_0} \approx r_{\text{Gauss}}$. 

As stated above, the resolution can in principle be improved beyond the divergence-limited resolution, i.e. below the waveguide diameter $d$ of a single-mode WG, by using scatter from the sample into angles larger than the waveguide divergence. However, the value of this improvement largely depends on the incident flux, sample scattering power and the waveguide width itself. To what extent this resolution gain below the waveguide dimension can be achieved by single-step holographic reconstruction rather than iterative reconstruction has to be further elucidated.

A technical limit to the obtainable resolution, especially if defocus distances $z > 1$ mm are used, can be set by the finite pixel size of the detector, i.e. one must assure that the diffraction pattern is sufficiently sampled. If the sample is illuminated by a plane wave with compact support and the detector is placed in the far field, the required oversampling ratio $\sigma_{os}$ has to obey $\sigma_{os} = \lambda z / (2 D \Delta) \geq 2$, where $D$ denotes the lateral extension of the illuminated area on the sample and $\Delta$ the detector pixel size. However, in the present situation object features corresponding to low spatial frequencies may still be imaged in the near field, while high-frequency components are mapped into the far field. The required oversampling ratio thus becomes dependent on the spatial frequencies of the object to be imaged. Generally, features with low spatial frequencies are more likely to be limited in resolution by the detector pixel size than high-frequency features.

The relation of WG cross-section and resolution is illustrated by the simulations shown in figure 4, carried out in the scheme described above, with the waveguide beam idealized by a Gaussian beam.

5. Numerical simulations and reconstructions

A simulated imaging experiment where the sample is scanned through the fixed WG illumination function $\psi_{ill}$ to increase the field of view is the basis of the reconstructions shown in figure 4: a Gaussian beam with $\Delta_{FWHM} = 75$ nm in vertical and horizontal direction in the WG exit plane, using $\Delta_{FWHM}$ as defined above, was assumed to propagate over a distance $z_1 = 0.9$ mm before impinging onto a test pattern with 500 nm thick Ta structure, illuminated with a photon energy of $E = 17.5$ keV. The expected phase shift and amplitude transmission of the Ta structure at the given parameters are $\Delta \phi = 0.40 \text{ rad}$ and $T = 0.96$, respectively. The contrast simulated here is identical to the expected contrast for the test object used in the physical experiment (see below). In view of the negligible absorption of unstained biological objects in a multi-keV x-ray beam, in the following we will concentrate on the reconstruction of the phase distribution only, as it strongly dominates the contrast formation mechanism even for heavy element materials. As a phantom object the well-known Siemens star design with controlled increase of spatial frequencies from the outer to the inner regions has been chosen. A quadratic scan with $10 \times 10$ scan points was simulated with a total flux of $1 \cdot 10^{7}$ photons per scan point impinging on the sample. The noisy diffraction signal was simulated to be measured at a distance of $z_2 = 3$ m from the sample on a quadratic detector area with a sidelength of 386 pixels and a pixel width of $55 \mu$m. To examine the effect of the source size on the resolution a second dataset was generated with $\Delta_{FWHM} = 25$ nm. The grid spacing of the scanning grid was adjusted to the size of the illuminating wave in the sample plane to allow for sufficient overlap between neighbouring scan positions (see below).

As a first step for the holographic reconstruction the coordinate transformation from divergent to parallel beam geometry was performed. Subsequently the simulated intensities
Figure 4. (a/b/d/e) Phase reconstructions (color bars in radians, scale bars denote 500 nm) obtained from simulated scanning holography/diffraction experiments, using a Gaussian beam as a model for waveguide illumination and an ideal Siemens star design for the object transmission function, with 20 continuous stripe pairs diverging from the center and a binary contrast equivalent to 500 nm Ta and air (vacuum). (c/f) Single simulated far field patterns out of the whole simulated scanning data used for corresponding reconstructions on the left (logarithmic scale, in photons per detector pixel). While holographic reconstruction was used in (a) and (d), the reconstructions shown in (b) and (e) were obtained by a ptychographic iterative method [6] from the same datasets as used in (a) and (d), respectively. The resolution is clearly improved by decreasing the source size from 75 nm (FWHM of intensity) in (a/b) to 25 nm (FWHM of intensity) in (d/e).

for each scan point were back-propagated to the sample plane. The individual complex-valued reconstructions were then added, in consideration of their respective positions, to yield the final object transmission. This ‘scanning holographic’ approach does not only provide an extended field of view beyond the lateral size of the waveguide beam on the sample, but also greatly decreases artifacts in the reconstructions coming from a non-ideal or fluctuating experimental illumination function. The phase distribution obtained by holographic reconstruction is shown in figure 4(a). The first zero of the phase contrast transfer function is predicted in $x$- and $y$-directions by equation (10) at a spatial half period (line or space width, respectively) of $L_{1/2} = 126$ nm. The ring with weakly inverted contrast at a spatial half period around 144 nm, visible in figure 4(a), (c) and partly also (d), is only in rough agreement with this value. More interestingly, structures with smaller spatial periods are reconstructed without zero contrast and with lowest artifacts, although the theory predicts an oscillating CTF with several additional spatial periods with zero contrast transfer down to the highest obtained resolution in the center. A possible explanation for this phenomenon might be connected to the nature of the Siemens
star pattern itself: For large radii the line pairs are parallel to a good approximation and the pattern more or less behaves like an isotropic analogue to 1D lines and spaces. However, with decreasing radii the line pairs become less and less parallel, so that in the central region the intrinsic 2-dimensional nature of the star pattern dominates, leading to unpredicted contrast behaviour in the framework of the 1D analogue of equation \((10)\), which has been used here.

An alternative route towards the reconstruction of the simulated holographic dataset has been opened up recently by an extended version of ptychographic diffractive imaging \([47]\). Here an iterative reconstruction method is applied which utilizes the Fourier transform relationship between the object exit wave and the measured far field intensity on the detector. More specifically, during each iteration the Fourier transform modulus of the current object exit wave is replaced by the measured Fourier amplitude to achieve consistency with the data (Fourier constraint). In addition, if positioned adequately, neighbouring scan positions will have overlapping illuminated areas, in which the exit waves have to be identical (real space constraint). While the first constraint is common to all iterative reconstruction methods in diffractive imaging, the latter is specific to ptychographic methods. Recently, several schemes have been presented to factorize the object exit wave at each scan position into the object transmission function and previously unknown complex illumination function in the sample plane \([6, 48, 49]\). It is thus possible to obtain the waveguide exit wave field by back-propagation of the sample illumination function to the waveguide exit plane.

Figure 4(b), obtained by ptychographic reconstruction of the same dataset as used in subfigure (a), shows improved resolution and image quality compared to the corresponding holographic reconstruction.

The image resolution was determined from fits of an error function to phase steps in circular line profiles. More precisely, the FWHM of the fitted error function’s derivative was defined as a measure for the resolution. Resolutions of \(r = 64\, \text{nm}\) (holographic reconstruction) and \(r = 31\, \text{nm}\) (ptychographic reconstruction) were obtained from the reconstructed phase distributions. The holographic resolution is in overall agreement with the expected value from Gaussian beam propagation, \(r_{\text{Gaussian}} = 1.33\Delta_{\text{FWHM}}\), considering that holographic signals below \(1/e\) times the maximum detected amplitude can easily contribute to the holographic reconstruction. The strong increase in resolution by ptychographic analysis is in good agreement with the observation that in the given geometry a substantial amount of scatter is directed outside the central cone of the waveguide exit wave, as visible in the simulated far field patterns on the detector (for an example out of the whole dataset, see figure 4(c)). In this case an iterative scheme based on an analysis of the full diffracted signal can strongly improve image resolution.

As expected, decreasing the source size from \(\Delta_{\text{FWHM}} = 75\, \text{nm}\) to \(25\, \text{nm}\) leads to an improved resolution in the holographic reconstruction (see figure 4(d)), namely \(r = 31\, \text{nm}\). Even though the waveguide far field is now better matched to the highest angles with sample scatter, as visible from the simulated intensities (see figure 4(f) for an example), the ptychographic reconstruction leads to an even higher resolution, below \(20\, \text{nm}\).

In summary, it cannot be generally stated that ptychographic iterative reconstruction will always improve the resolution as substantially as in this case, especially in the case of weakly scattering biological samples. However, the present analysis shows that for holographic reconstruction the far field pattern of the waveguide exit wave should be adjusted to the sample scattering angle at the given flux. In addition, due to the strong decay of scattering signal with increasing scattering angle, increasing the resolution by diffractive (ptychographic) analysis with smaller and smaller source sizes becomes more and more difficult.
Notably, according to the standard oversampling condition of plane-wave CDI (see above) the maximum allowed extension of the illumination function in the sample plane to achieve an oversampling ratio \( \sigma_{\text{os}} > 2 \) is given here as \( D_{\text{min}} = 0.97 \mu \text{m} \). For the second simulated dataset \( (\Delta_{\text{FWHM}} = 25 \text{ nm}) \) this is substantially below the \( 1/e \)-FWHM of the simulated amplitude, i.e. \( D_{1/e} = 1.91 \mu \text{m} \).

Which constraints and restrictions apply to holographic reconstruction and how does it compare to CDI in parallel beams? First of all, as a variant of propagation imaging, the spatial frequencies, for which the CTF is zero, are not properly transmitted, and the reconstruction will lack the corresponding Fourier components, unless information from several well chosen defocus distances is combined [13]. The coherence and monochromaticity requirements are addressed in [43], and can be relaxed in the regime of direct imaging, enabling high flux pink beam measurements. Compared to CDI, the use of a beamstop and the associated problems are obsolete in projection holography due to the spreading of the direct beam onto many detector pixels. In this sense holography makes better use of state-of-the-art detectors than diffraction imaging. It also enables a deterministic single-step reconstruction in real time. Reconstruction schemes taking into account the exact phase fronts of the empty beam beyond the point source approximation may further help to increase image quality and eventually also resolution. The use of support constraints and, as presented above, a combination of holographic and iterative algorithms, which are well established in CDI, can be combined with holographic reconstruction [36], and applied to the current imaging scheme.

6. Recent experimental results

In the following we report on an experiment performed at the ID22-NI undulator beamline at the third generation synchrotron facility ESRF (Grenoble, France). Two undulators were used simultaneously, working at the second and fifth harmonic, respectively. The radiation was used in the so-called pink mode (no crystal monochromators) at a photon energy of \( E = 17.5 \text{ keV} \), using the intrinsic monochromaticity of the undulators and the bandpass of the multilayer KB mirror system, resulting in \( \Delta \lambda / \lambda \simeq 0.02 \). In addition, a flat horizontally deflecting Pd-coated Si-mirror was used at 0.15° incidence angle for higher harmonics rejection. The focus of the KB-mirrors was characterized by translation of an Au stripe, recording both the transmitted intensity by a diode and the Au L\(_{\text{α}}\) fluorescence by a silicon drift detector (Vortex-EX, SII NanoTechnology Inc.). The measured focal spot size was \( D_{\text{horz}} = 129 \text{ nm} \) (FWHM of fluorescence intensity) in the horizontal and \( D_{\text{vert}} = 166 \text{ nm} \) (FWHM of fluorescence intensity) in the vertical direction, respectively. The total intensity in the focal spot was on the order of \( 10^{11} \text{ ph s}^{-1} \), depending on the ring current and the slit settings in front of the KB.

A bonded-2DWG was aligned in terms of three translations and two rotations (Attocube Systems, Germany) in the focal plane of the KB. The waveguide structure itself consisted of 13 mm long air channels (lateral dimensions 140 nm (hor.) \( \times \) 24 nm (vert.)) in a bonded Si structure. To facilitate the alignment procedure multiple channels of the same dimensions were arranged in parallel, 400 nm apart from each other. Before the experiment a single channel was placed into the focus of the KB mirror, yielding a total flux exiting the waveguide on the order of \( 10^{10} \text{ ph s}^{-1} \), as measured on the 2D detector.

For the imaging experiment, a high resolution chart (NTT-AT, Japan, model # ATN/XRESO-50HC) consisting of a 500 nm thick nanostructured Ta layer on a SiC membrane was placed in the beam at a distance of \( z_1 = 0.926 \text{ mm} \) from the crossed 2DWG, as determined...
Figure 5. Diffraction patterns of the Siemens star test pattern recorded for different imaging regimes: holographic projection imaging with waveguide illumination at (a) large defocus $z \approx 22$ mm (ID1/ESRF, $E = 8$ keV, bonded-2DWG: $\ell = 1.3$ mm, 250 (hor.) $\times$ 35 (vert.) nm$^2$ guiding channel) and (b) small defocus $z = 0.926$ mm (ID22/ESRF, $E = 17.5$ keV, bonded-2DWG: $\ell = 13$ mm, 140 (hor.) $\times$ 24 (vert.) nm$^2$ guiding channel), with correspondingly large and small field of view, respectively. (c) Pinhole illumination (cSAXS/SLS, $E = 6.2$ keV, pinhole drilled in W-foil by FIB: $\ell = 20$ $\mu$m, diameter $d = 1.4$ $\mu$m), distance between pinhole and sample, 1.4 mm, distance between sample and detector, 7.22 m. A scanning electron micrograph showing the central region of the Siemens star test pattern is depicted in (d). Note that in contrast to the design used for simulation the radial stripes diverging from the center are separated into rings of defined spatial period at the innermost radius (50 nm line width at the beginning of the central (first) ring, 100 nm line width at the beginning of the second ring, 200 nm at the third ring).

optically with a microscope coaxial with the optical axis (Accel, Germany). A low noise direct photon counting pixel detector (Maxipix, ESRF [50]) with a pixel size of 55 $\mu$m and an active area of $256 \times 256$ pixels was used to image the in-line hologram at a distance $z_2 = 3.09$ m from the sample. The effective defocus distance $z$ as defined above was thus $z = 0.923$ mm with a geometric magnification factor of $M = 334$. To increase the field of view the sample was scanned through the beam on a rectangular grid with a spacing of 250 nm in the plane perpendicular to the optical axis. A total number of $21 \times 21$ diffraction patterns was collected with an illumination time of 1 s per scan point.

Figure 5 shows the holograms and far field diffraction patterns of the Siemens star test object recorded under different imaging conditions, as detailed in the caption (for movies showing whole scans see supporting material, available at stacks.iop.org/NJP/12/035008). Figure 5(b) was obtained in the geometry described above. The strong magnification effect with decreasing defocus distance $z$ is clearly visible in (a) and (b). While the divergent waveguide illumination leads to a spread of the illumination function on the whole area of the detector and a holographic image of the object structure, the nearly parallel illumination by a comparatively large pinhole (1.4 $\mu$m diameter) causes a typical Airy pattern with a strong central peak on the detector figure 5(c). As a consequence, a high dynamic range is necessary here to record both the central maximum and the modulations of the far field intensity by the object transmission function, which show no resemblance to the real space structure any more.
Phase reconstructions of the object transmission function corresponding to the dataset shown in figure 5(b), obtained both by iterative and holographic reconstruction, are shown in figures 6(a) and (c), respectively.

For the analysis all diffraction patterns were normalized to their average intensity to remove slight drift in the waveguide intensity originating from variation in ring current as well as nanometer-range positional drift in the setup. The holographic reconstruction was obtained in the same way as described above for simulated datasets. For the ptychographic reconstruction the scheme demonstrated in [6] was used, which utilizes the difference map algorithm for application of the Fourier space constraint [51]. To avoid drifts in the algorithmic reconstruction the difference map was exchanged with the error reduction algorithm after the first 10 iterations. This algorithm is known as a local optimizer and has been used in a recently presented extended version [49] of the original ptychographic scheme [47]. The reconstruction shown in figure 6(a) was obtained after a total number of 40 iterations.

Figure 6. Iterative (top) and holographic (bottom) reconstructions of the object transmission function (phase) of a Siemens star test pattern illuminated with a bonded 2-dimensional waveguide. The insets (b/d) in the middle were magnified from the reconstructed images shown on the left (a/c). Line scans (white/black) through the phase distributions shown in (b) and (d) and corresponding fits (red) of Gaussian error functions to single phase steps are shown on the right. Scale bars in (a) and (c) denote 1 µm. All phase values are given in rad.
While the overall structure of the test pattern is recovered up to very fine details in the center region with both reconstruction methods, the retrieved phase values are only in coarse agreement with the expected phase shift of 0.4 rad between the void areas (high phase values) and the Ta structure (lower, retarded phase values). In the ptychographic reconstruction the retrieved phase difference between filled and void areas is generally smaller than the expected value, the situation is reversed in the holographic reconstruction. This phenomenon is also visible in the reconstruction of simulated data shown in figure 4. The holographic reconstruction also shows stronger artifacts and non-reconstructed spatial frequencies which are due to the non-uniform phase contrast transfer function as described above. In general this behaviour is very similar to what has been observed for reconstructions from simulated data (see section 5). Note that here the true pattern itself (see figure (d)) is separated into distinct rings with a defined range of spatial frequencies, with non-patterned areas in between the rings.

As visible in both types of reconstructions the spatial resolution is higher in vertical than in horizontal direction. There is a direct correspondence between this anisotropy and the lateral dimensions of the waveguide guiding core (140 nm (hor.) × 24 nm (vert.)), which strongly confines the guided field in the vertical direction with milder confinement in the horizontal direction.

The highest obtained resolution, in the vertical direction, was estimated as described for the simulated datasets. For the holographic reconstruction a value of \( r = 36 \text{ nm} \) (FWHM) was obtained, the ptychographic reconstruction yields \( r = 34 \text{ nm} \) (FWHM). In contrast to the reconstructions from simulated data, the gain in resolution by ptychographic analysis is not as high. This could be connected to vibrations and long term drift of the sample with respect to the beam, as well as limited spatial coherence.

As described before, the ptychographic scheme allows for a reconstruction of the wave field illuminating the sample, and by free space back-propagation, also of the waveguide exit wave field. The waveguide exit wave intensity, back-propagated from the reconstructed object illumination function over a distance \( z = 0.92 \text{ mm} \), is shown in figure 7. Gaussian fits to the central intensity peak yield a FWHM of 29 nm (horizontal) and 17 nm (vertical). Both values indicate field confinement to much smaller values than the respective channel width (140 nm (hor.) × 24 nm (vert.)). This is in good agreement with the FD simulations carried out to study the wave field inside the guiding core (see section 3).

A comparison of the exit wave size to the reconstructed resolution shows that, in contrast to reconstructions from simulated data, the minimum resolved lengthscale is larger than the measured size of the WG exit wave. It is noted here that on these lengthscales limited longitudinal coherence of the pink beam \[43\], as well as sample vibrations and drift could alter the maximum possible resolution quite substantially.

As evaluated from the reconstruction, the maximum flux density at the waveguide exit was \( 7.3 \cdot 10^9 \text{ph/s/\mu m}^2 \). The finite background level of the reconstructed intensity \( (I_{bg} = 4.3 \cdot 10^3 \text{ph/s/\mu m}^2) \) indicates a finite transmission of the waveguide cladding \((\ell = 13 \text{ mm Si along the optical axis})\), given the high incident flux impinging on the waveguide entrance.

7. Outlook and conclusions

In summary, we have shown the successful application of two-dimensionally confining x-ray waveguides to high-resolution imaging of extended specimens at multi-keV photon energies, down to a spatial resolution below 50 nm. The image formation and reconstruction process was
Figure 7. (a) Reconstructed intensity (logscale colorbar in units of \( \text{ph} \mu \text{m}^{-2} \text{s}^{-1} \)) in the waveguide exit plane. The horizontally periodic structure (period length 400 nm) of the waveguide arrangement inside the Si cladding is very well reproduced, indicating a leakage of air-scattered photons into the neighbouring WG channels. A mean background intensity of \( 4.3 \times 10^3 \text{ph} \mu \text{m}^{-2} \text{s}^{-1} \) was obtained in the area marked by a white square. (b/c) Line scans and Gaussian fits along the symmetry axes of the WG exit intensity in horizontal (a) and vertical direction (b).

studied both for simulated and experimental data. Two independent analysis approaches were followed and successfully applied: single-step holographic back-projection and diffraction-based ptychographic iterative reconstruction. It was found by analytical estimations as well as reconstructions from simulated data that for holographic phase retrieval the resolution is limited to a good approximation by the size of the source which is idealized as a point source in the present scheme of holographic reconstruction. Reconstructions from simulations have shown the potential of ptychographic analysis to increase the resolution beyond the limit currently set by holographic reconstruction. This increase is clearly connected to the scattering power of the sample and the ratio of the waveguide divergence and the highest angle where scattering from the sample is detected. Consequently, the waveguide divergence should be adjusted to the expected exit cone where sample scattering is expected. In a more general sense, waveguide optics offers design parameters that can be adjusted to optimize the illumination function with respect to sample specification and reconstruction schemes. Moreover, the limited dynamic range of state-of-the-art detectors is better utilized by divergent than by parallel beams. It was found both in simulations and experimentally that iterative ptychographic analysis can push forward the accuracy of reconstructed phase values with respect to holographic reconstruction, which is, however, based on a single-step calculation which can be performed in real time. This is also relevant for possible extensions of the method to 3D (tomographic) imaging. Furthermore, a holographic reconstruction from simulated data has shown the potential of the method to image unstained biological objects (cells, tissues) under identical imaging conditions (photon energy, geometric magnifications) with resolutions well into the sub-100 nm range. A dedicated setup for the range of applications presented here is currently under construction at New Journal of Physics 12 (2010) 035008 (http://www.njp.org/)
Figure 8. Schematic of dedicated instrumentation and sample preparation for waveguide based holography of biological samples (under construction for the P10 beamline at PETRA III). (a/b) A KB focusing system is used to focus the highly coherent undulator beam onto the entrance of a two-dimensionally confined waveguide or directly onto the sample. A cryogenic sample environment using a jet of nitrogen gas is available to reduce beam damage. The sample which is placed on a thin Kapton foil (d) can be visualized during exposure with x-rays using a microscope with a drilled lens to allow passage of the x-ray beam. An optical micrograph obtained with the in situ microscope under cryogenic conditions shows frozen-hydrated *Dictyostelium discoideum* cells (c). The detector, either a direct illuminated CCD or a single-photon counting pixel detector, is placed 6 m downstream of the sample. (e/f) Preparation of biological samples (details can be found in [52]). After adhesion of the living cells to the Kapton film the sample holder is injected into liquid ethane to prevent crystallization of the water surrounding the sample. Afterwards the sample can be directly used for imaging (under cryogenic conditions) or further processed by freeze-drying.

the P10-‘Coherence’-beamline of the new synchrotron source PETRA III at DESY (Hamburg, Germany), see figure 8. Together with the analytical tools presented here this opens up a route to multi-modal quantitative high resolution imaging of extended and unstained biological samples.

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